WEST Search History

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DATE: Friday, November 24, 2006

Hide?	Set Name	Query	Hit Count
	DB=PGPB; PLUR=YES; OP=ADJ		
☐	L4	l3 and integrin.CLM.	11
☐	L3	l2 and inflammat$.CLM.	226
☐	L2	l1 and (amine or amino or pyrrolidin$ or pyrrol$ or piperidin$ or pyridin$.CLM.)	1189
☐	L1	phenylpropionic acid or phenylpropionic acid derivative.CLM.	1221

END OF SEARCH HISTORY

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=> d his

     (FILE 'HOME' ENTERED AT 12:21:07 ON 24 NOV 2006)

     FILE 'REGISTRY' ENTERED AT 12:21:27 ON 24 NOV 2006
L1             STRUCTURE UPLOADED
L2               7 S L1
L3              53 S L1 FULL

     FILE 'HCAPLUS, CHEMCATS' ENTERED AT 12:22:29 ON 24 NOV 2006
L4              26 S L3

     FILE 'HCAPLUS, HCAOLD, USPATFULL, EPFULL, MEDLINE, BIOSIS' ENTERED AT
     12:34:43 ON 24 NOV 2006
L5            7351 S PHENYLPROPIONIC ACID OR PHENYLPROPIONIC ACID DERIVATIVE?
L6            1527 S L5 AND INFLAMMAT?
L7             131 S L6 AND INTEGRIN
L8             127 S L7 AND (MEDICINE OR MEDICAMENT OR PHARMACEUTICAL)
L9             127 S L8 AND (AMINE OR AMINO OR HETEROCYCLIC OR HETEROCYCLE)
L10             84 S L9 AND PYRROLIDIN?
L11             84 S L10 AND PYRROL?
L12             80 S L11 AND PIPERIDIN?
L13             80 S L12 AND PYRIDIN?
L14             24 S L13 AND CYTOSIN?
L15             21 S L14 AND (ARTHRITIS OR LUPIS OR MULTIPLE SCHLEROSIS OR ASTHMA
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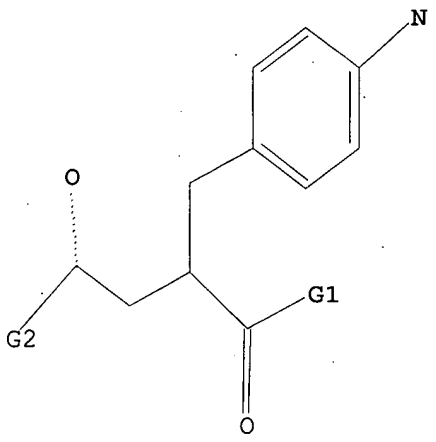
L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 OH,N,MeO,EtO,n-PrO,n-BuO

G2 Cb,Hy,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 12:21:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 96 TO ITERATE

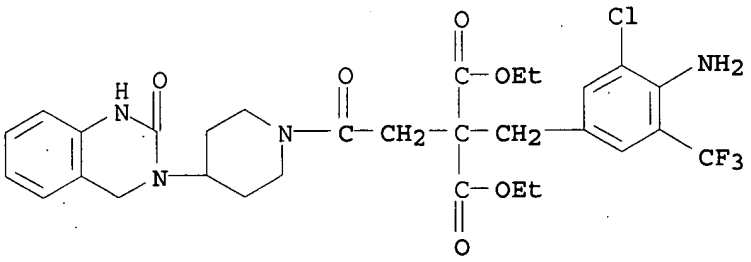
100.0% PROCESSED 96 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1333 TO 2507
PROJECTED ANSWERS: 7 TO 298

L2 7 SEA SSS SAM L1

=> d scan

L2 7 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Propanedioic acid, [[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl][2-[4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-1-piperidinyl]-2-oxoethyl]-, diethyl ester (9CI)
MF C30 H34 Cl F3 N4 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

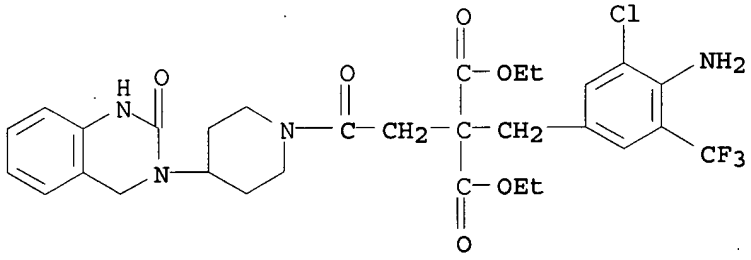
=> s l1 full
FULL SEARCH INITIATED 12:22:00 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1907 TO ITERATE

100.0% PROCESSED 1907 ITERATIONS 53 ANSWERS
SEARCH TIME: 00.00.01

L3 53 SEA SSS FUL L1

=> d scan

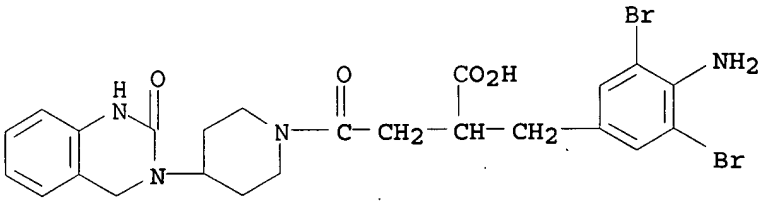
L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Propanedioic acid, [[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl][2-[4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-1-piperidinyl]-2-oxoethyl]-, diethyl ester (9CI)
MF C30 H34 Cl F3 N4 O6



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):10

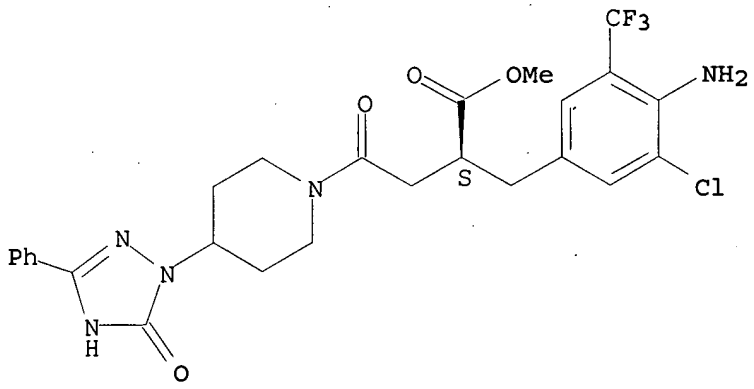
L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Piperidinebutanoic acid, α-[(4-amino-3,5-dibromophenyl)methyl]-4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-γ-oxo- (9CI)
MF C24 H26 Br2 N4 O4



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

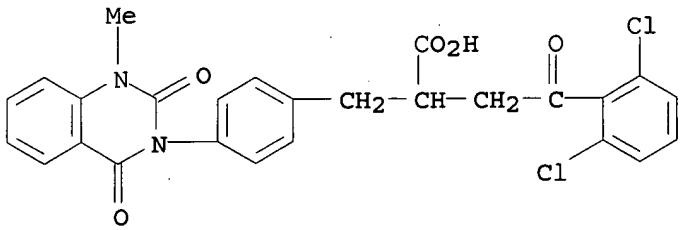
L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(2,5-dihydro-5-oxo-3-phenyl-1H-1,2,4-triazol-1-yl)-γ-oxo-, methyl ester, (αS)- (9CI)
MF C26 H27 Cl F3 N5 O4

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

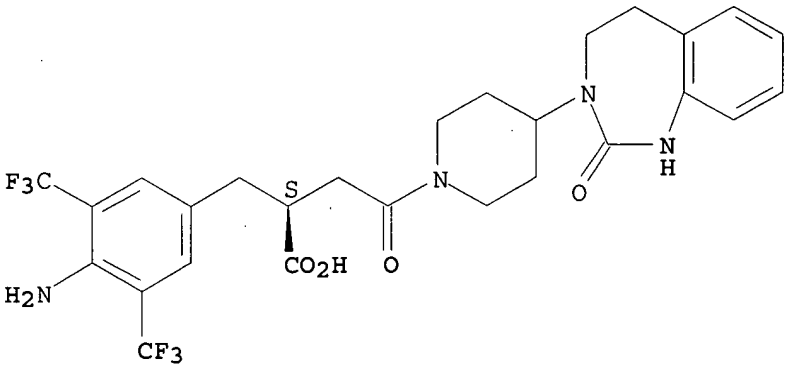
L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenebutanoic acid, 2,6-dichloro-α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo- (9CI)
MF C26 H20 Cl2 N2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

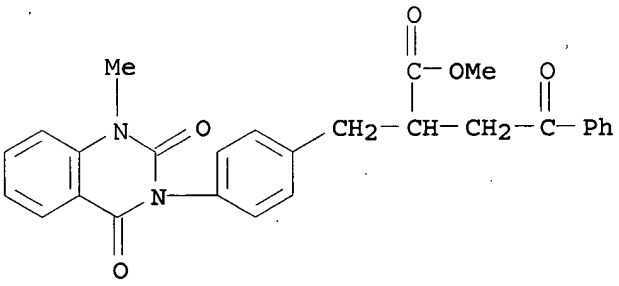
L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Piperidinebutanoic acid, α-[[4-amino-3,5-bis(trifluoromethyl)phenyl]methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI)
MF C27 H28 F6 N4 O4

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

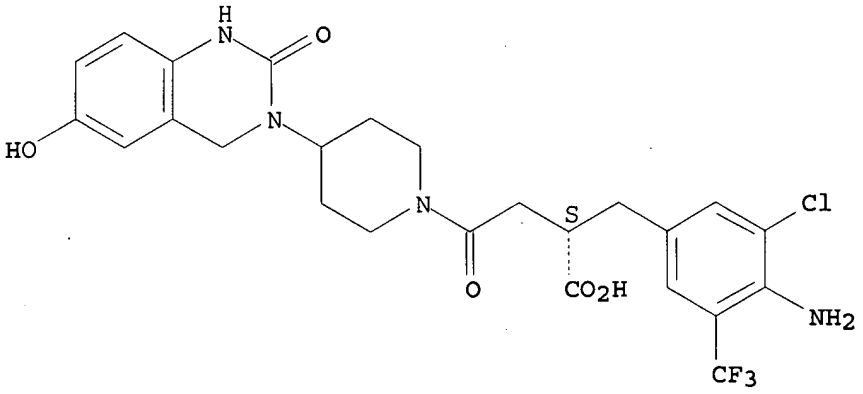
L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Benzenebutanoic acid, α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo-, methyl ester (9CI)
MF C27 H24 N2 O5



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,4-dihydro-6-hydroxy-2-oxo-3(2H)-quinazolinyl)-γ-oxo-, (αS)- (9CI)
MF C25 H26 Cl F3 N4 O5

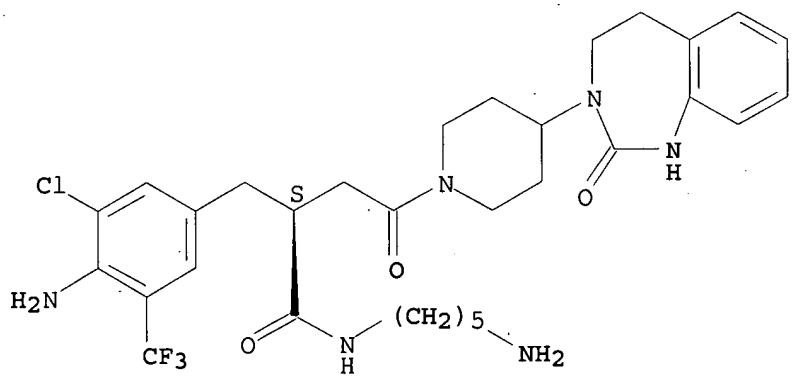
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Piperidinebutanamide, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-N-(5-aminopentyl)-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI)
MF C31 H40 Cl F3 N6 O3

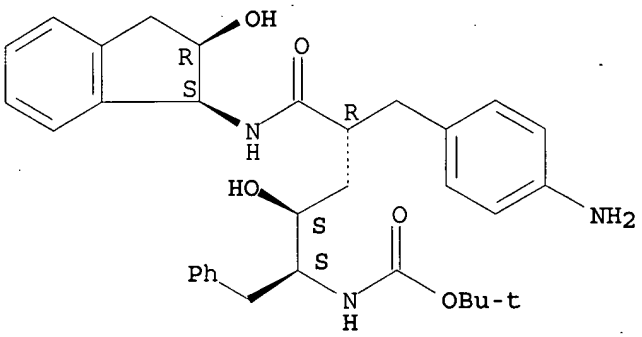
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI)
MF C33 H41 N3 O5

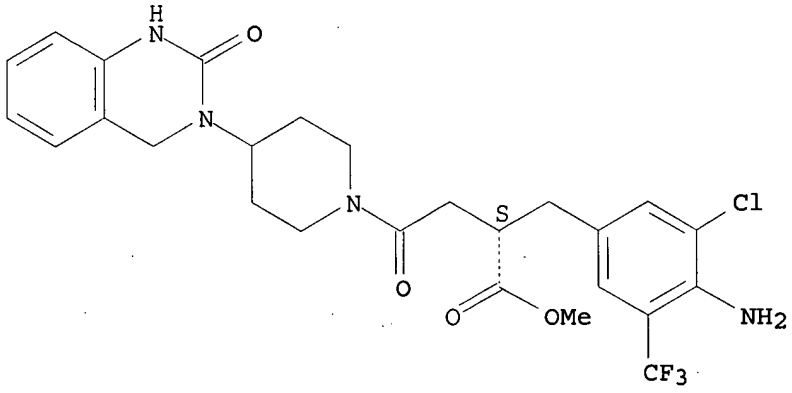
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-γ-oxo-, methyl ester, (αS)- (9CI)
MF C26 H28 Cl F3 N4 O4

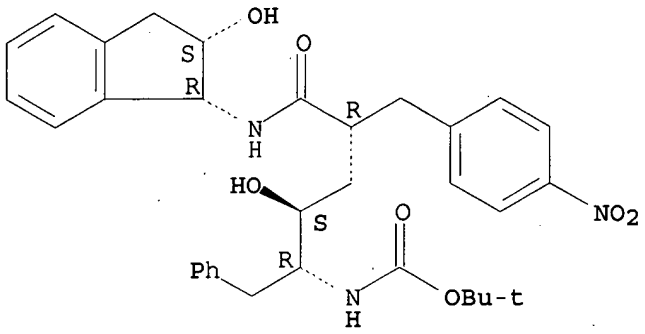
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 53 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN Carbamic acid, [(1R,2S,4R)-5-[[(1R,2S)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI)
MF C33 H39 N3 O7

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> file hcaplus chemcat

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	167.38	167.59

FILE 'HCAPLUS' ENTERED AT 12:22:29 ON 24 NOV 2006
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=> s l3
L4 26 L3

=> d 0-26 ibib abs hitstr
'0-26' IS NOT A VALID FORMAT FOR FILE 'HCAPLUS'

The following are valid formats:

ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
BIB --------- AN, plus Bibliographic Data and PI table (default)
CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
SCAN must be entered on the same line as the DISPLAY,
e.g., D SCAN or DISPLAY SCAN)

STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT) containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its structure diagram, plus NTE and SEQ fields
KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.
ENTER DISPLAY FORMAT (BIB):end

=> d 1-26 ibib abs hitstr

L4 ANSWER 1 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:1005390 HCAPLUS
DOCUMENT NUMBER: 145:356814
TITLE: Preparation of 2-oxo-1,2,4,5-tetrahydro-1,3-benzodiazepin-3-ylpiperidines and related compounds as CGRP receptor antagonists
INVENTOR(S): Mueller, Stephan Georg; Rudolf, Klaus; Lustenberger, Philipp; Stenkamp, Dirk; Santagostino, Marco; Paleari, Fabio; Doods, Henri; Arndt, Kirsten; Schaenzle, Gerhard
PATENT ASSIGNEE(S): Boehringer Ingelheim International G.m.b.H., Germany; Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G.
SOURCE: PCT Int. Appl., 231pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006100009	A1	20060928	WO 2006-EP2515	20060318
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WO 2005092880	A1	20051006	WO 2005-EP3094	20050323
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WO 2005103037	A2	20051103	WO 2005-EP4104	20050418
WO 2005103037	A3	20060112		
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			WO 2005-EP4104	A 20050418
			EP 2005-21283	A 20050929
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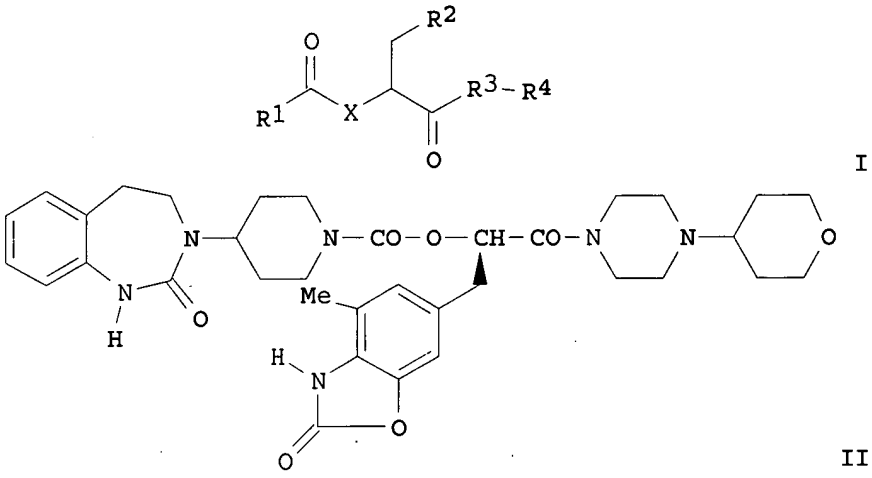
OTHER SOURCE(S):	MARPAT 145:356814			

GI



I

II

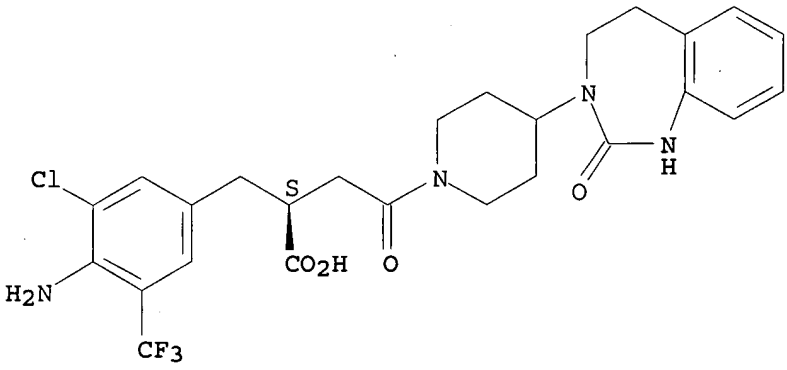
AB Title compds. I [X = CH2, NH, O, etc.; R1 = substituted 2-oxo-1,2,4,5-tetrahydro-1,3-benzodiazepin-3-ylpiperidines, etc.; R2 = 5-methylquinoxalines, 8-methylimidazo[1,2-a]pyridines, etc.; R3 = substituted piperidines, piperazines, etc.; R4 = 4 to 7-membered ocicycloalkyl ring with provisos] and their pharmaceutically acceptable salts and formulations were prepared For example, benzodiazepinylpiperidine II was prepared from 5-amino-m-cresol in 8-steps. In CGRP receptor inhibition assays, compds. I exhibited IC50 values ≤ 10000 nM.

IT 688020-76-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of oxotetrahydrobenzodiazepinylpiperidines and related compds. as CGRP receptor antagonists)

RN 688020-76-0 HCAPLUS

CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



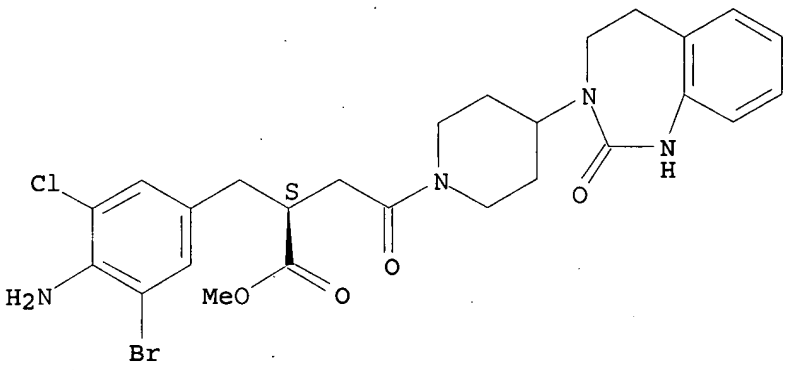
IT 910575-90-5P 910575-91-6P 910575-92-7P
910576-03-3P 910576-04-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of oxotetrahydrobenzodiazepinylpiperidines and related compds. as CGRP receptor antagonists)

RN 910575-90-5 HCAPLUS

CN 1-Piperidinebutanoic acid, α-[(4-amino-3-bromo-5-

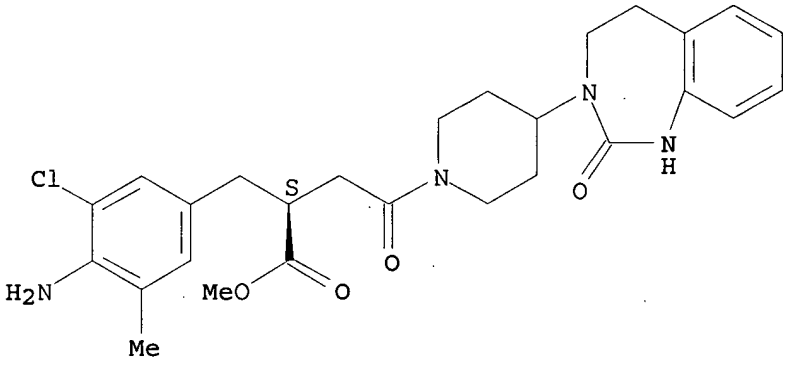
chlorophenyl)methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



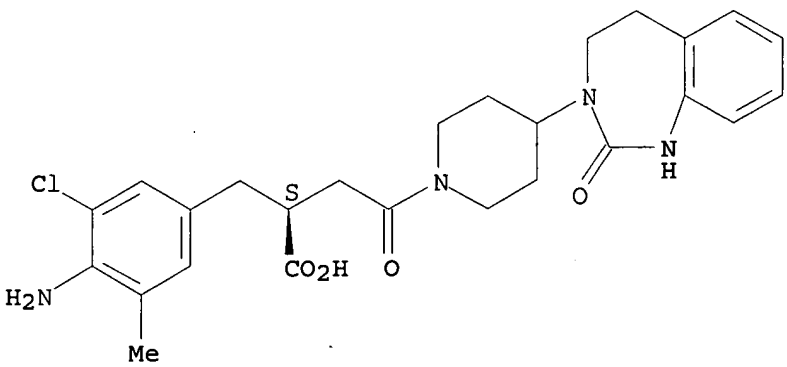
RN 910575-91-6 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[(4-amino-3-chloro-5-methylphenyl)methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



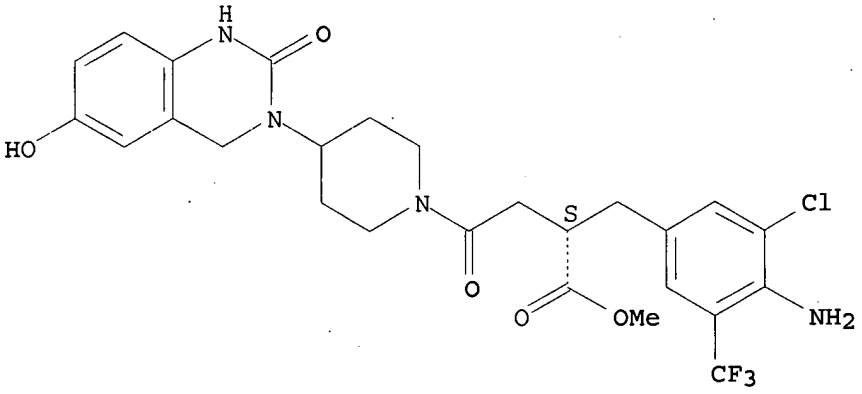
RN 910575-92-7 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[(4-amino-3-chloro-5-methylphenyl)methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



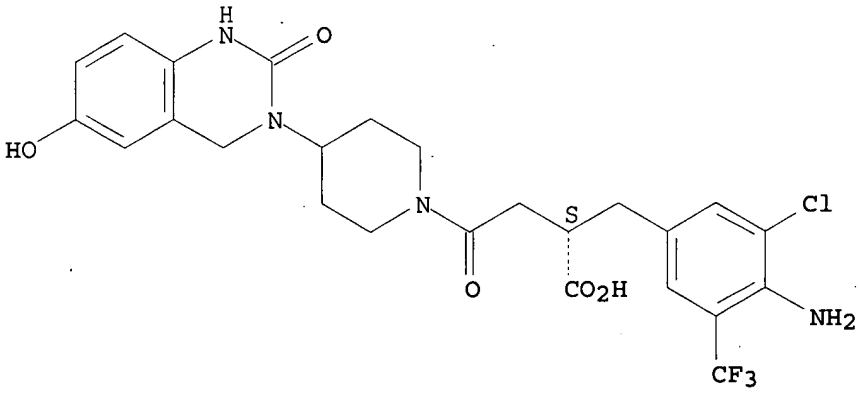
RN 910576-03-3 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,4-dihydro-6-hydroxy-2-oxo-3(2H)-quinazolinyl)-γ-oxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 910576-04-4 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,4-dihydro-6-hydroxy-2-oxo-3(2H)-quinazolinyl)-γ-oxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:44967 HCAPLUS
DOCUMENT NUMBER: 144:205230
TITLE: Probabilistic Neural Network Model for the In Silico Evaluation of Anti-HIV Activity and Mechanism of Action
AUTHOR(S): Vilar, Santiago; Santana, Lourdes; Uriarte, Eugenio
CORPORATE SOURCE: Faculty of Pharmacy, Department of Organic Chemistry, University of Santiago de Compostela, Santiago de Compostela, 15782, Spain
SOURCE: Journal of Medicinal Chemistry (2006), 49(3), 1118-1124

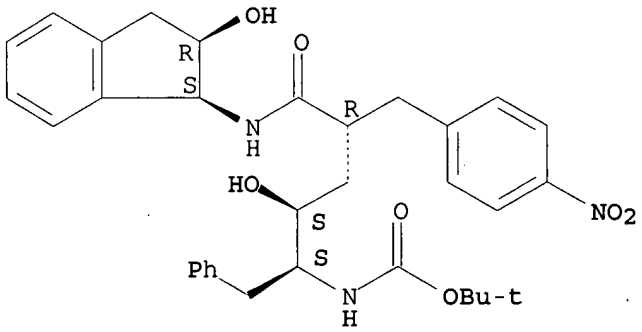
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A theor. model has been developed that discriminates between active and nonactive drugs against HIV-1 with four different mechanisms of action for the active drugs. The model was built up using a probabilistic neural network (PNN) algorithm and a database of 2720 compds. The model showed an overall accuracy of 97.34% in the training series, 85.12% in the selection series, and 84.78% in an external prediction series. The model not only correctly classified a very heterogeneous series of organic compds. but also discriminated between very similar active/nonactive chems. that belong to the same family of compds. More specifically, the model recognized 96.02% of nonactive compds., 94.24% of active compds. that inhibited reverse transcriptase, 97.24% of protease inhibitors, 97.14% of virus uncoating inhibitors, and 90.32% of integrase inhibitors. The results indicate that this approach may represent a powerful tool for modeling large databases in QSAR with applications in medicinal chemical

IT 126410-15-9 126410-17-1
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(probabilistic neural network model for In silico evaluation of anti-HIV activity and mechanism of action)

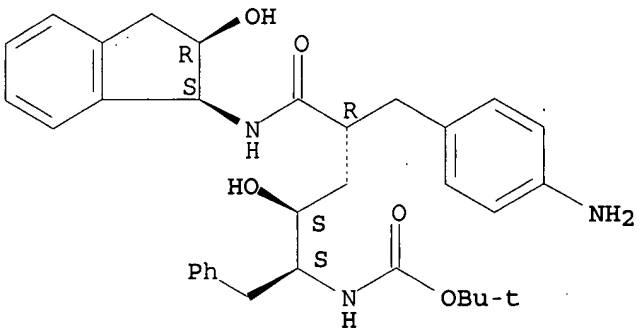
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 80 THERE ARE 80 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:587914 HCAPLUS
DOCUMENT NUMBER: 141:140319
TITLE: Preparation of amino acid dipiperidides as CGRP antagonists
INVENTOR(S): Bauer, Eckhart; Gerlach, Kai; Hurnaus, Rudolf; Mueller, Stephan; Rudolf, Klaus; Schindler, Marcus; Stenkamp, Dirk
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. KG, Germany
SOURCE: Ger. Offen., 98 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10300973	A1	20040722	DE 2003-10300973	20030114
AU 2004203916	A1	20040729	AU 2004-203916	20040109
CA 2513132	AA	20040729	CA 2004-2513132	20040109
WO 2004063171	A1	20040729	WO 2004-EP87	20040109
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA				
EP 1587795	A1	20051026	EP 2004-700987	20040109
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2004006762	A	20051220	BR 2004-6762	20040109
CN 1738805	A	20060222	CN 2004-80002209	20040109
JP 2006515875	T2	20060608	JP 2006-500537	20040109
US 2004192729	A1	20040930	US 2004-755593	20040112
NO 2005003794	A	20050810	NO 2005-3794	20050810
PRIORITY APPLN. INFO.:			DE 2003-10300973 A	20030114
			US 2003-443492P P	20030129
			WO 2004-EP87 W	20040109

OTHER SOURCE(S): MARPAT 141:140319
GI

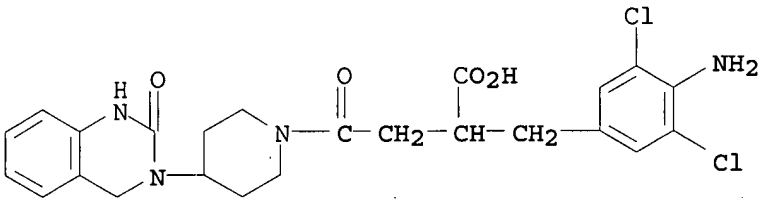
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R = (un)substituted diaza-, triaza-, S,S-dioxidothiadiaza-heterocycle; Ar = (un)substituted aryl, heteroaryl; Y = CH2, NH; Y1 = (un)substituted CH, N; R1 = (un)substituted N heterocycle; R2, R3 = H, carboxylic ester] were prepared for use as CGRP antagonists in the production and purification of antibodies and as marked compds. in RIA and ELISA assays and as diagnostic or analytic additives in neurotransmitter research (no data). Thus, the piperidide II was prepared from the amino acid and piperidine fragments in a multi-step synthesis.

IT 726184-84-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino acid dipiperidides as CGRP antagonists)

RN 726184-84-5 HCAPLUS

CN 1-Piperidinebutanoic acid, α-[(4-amino-3,5-dichlorophenyl)methyl]-4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-γ-oxo- (9CI) (CA INDEX NAME)



L4 ANSWER 4 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:370922 HCAPLUS

DOCUMENT NUMBER: 140:391301

TITLE: Preparation of benzo-1,3-diazepin-2-ones and related compounds as CGRP receptor antagonists for the treatment of migraine headaches

INVENTOR(S): Rudolf, Klaus; Mueller, Stephan Georg; Stenkamp, Dirk; Lustenberger, Philipp; Dreyer, Alexander; Bauer, Eckhart; Schindler, Marcus; Kirsten, Arndt; Doods, Henri

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G., Germany

SOURCE: PCT Int. Appl., 315 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037810	A1	20040506	WO 2003-EP11762	20031023
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10250080	A1	20040513	DE 2002-10250080	20021025
US 2006079504	A1	20060413	US 2003-687262	20031016
CA 2503455	AA	20040506	CA 2003-2503455	20031023

AU 2003276156	A1	20040513	AU 2003-276156		20031023
EP 1558600	A1	20050803	EP 2003-809317		20031023
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
BR 2003015665	A	20050830	BR 2003-15665		20031023
CN 1708493	A	20051214	CN 2003-80102004		20031023
JP 2006516244	T2	20060629	JP 2004-545963		20031023
NO 2005002496	A	20050624	NO 2005-2496		20050524
PRIORITY APPLN. INFO.:			DE 2002-10250080	A	20021025
			US 2002-426168P	P	20021114
			WO 2003-EP11762	W	20031023

OTHER SOURCE(S): MARPAT 140:391301
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

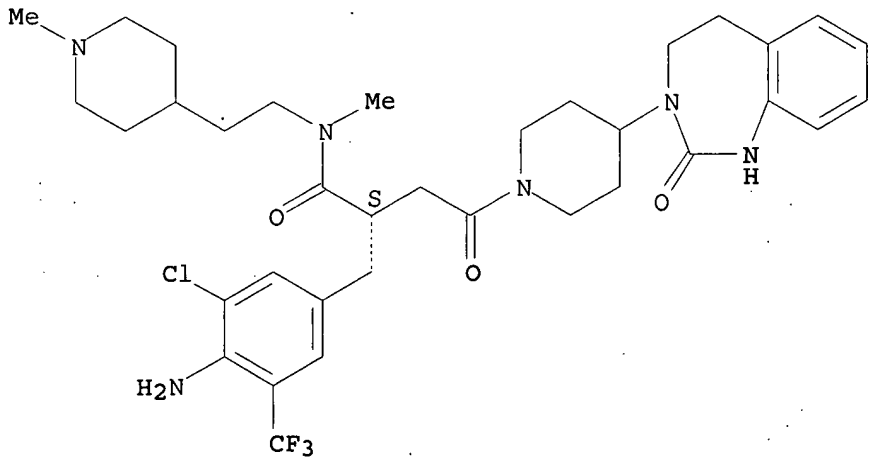
AB Title compds. I [A = O, S, phenylsulfonylimino, etc.; X = O, S, substituted imino, etc.; U = alkyl, alkenyl, alkynyl, etc.; V = Cl, Br, amino, etc.; W = H, halo, difluoromethyl, etc.; R1 = 5-7 membered aza, diaza, triaza, etc. heterocycle; R2 = H, phenylmethyl, alkyl, etc.; R3 = H, Ph, pyridinyl, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, benzo-1,3-diazepin-2-one II was prepared from 4-amino-3-chloro-5-trifluoromethylbenzoic acid in 9-steps. In human CGRP receptor binding affinity assays, compds. I exhibited IC50 values < 10000 nM. Compds. I are claimed useful for the treatment of migraine headaches.

IT 688018-74-8P 688018-75-9P 688019-09-2P
688019-10-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzo-1,3-diazepin-2-ones and related compds. as CGRP receptor antagonists for the treatment of migraine headaches)

RN 688018-74-8 HCAPLUS

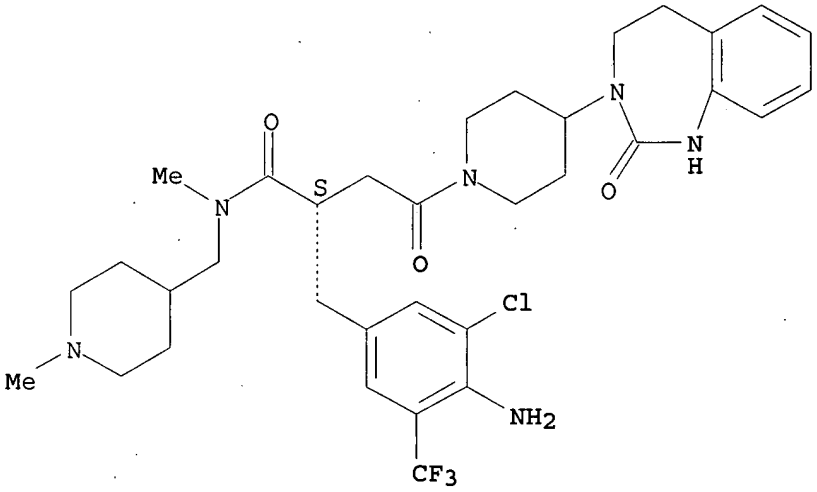
CN 1-Piperidinebutanamide, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-N-methyl-N-[2-(1-methyl-4-piperidinyl)ethyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



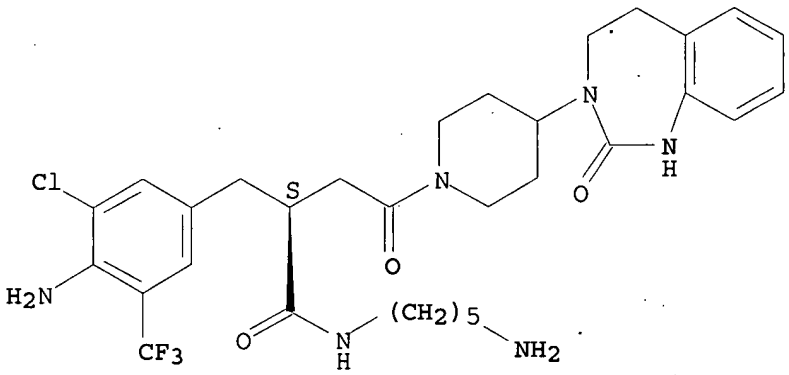
RN 688018-75-9 HCAPLUS
CN 1-Piperidinebutanamide, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-N-methyl-N-[(1-methyl-4-piperidinyl)methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



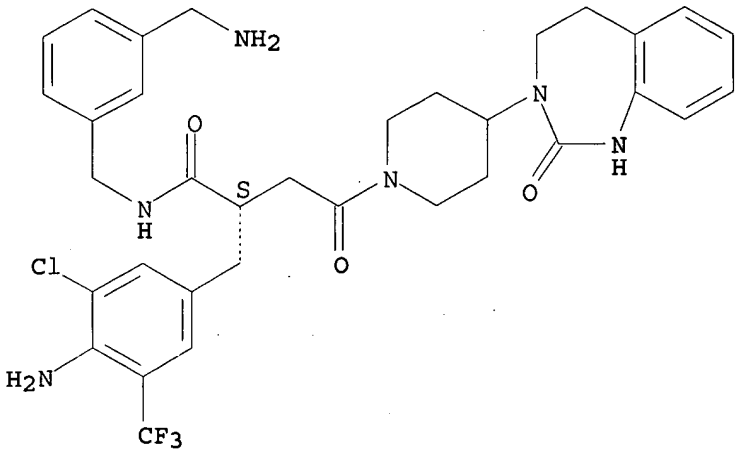
RN 688019-09-2 HCAPLUS
CN 1-Piperidinebutanamide, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-N-(5-aminopentyl)-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



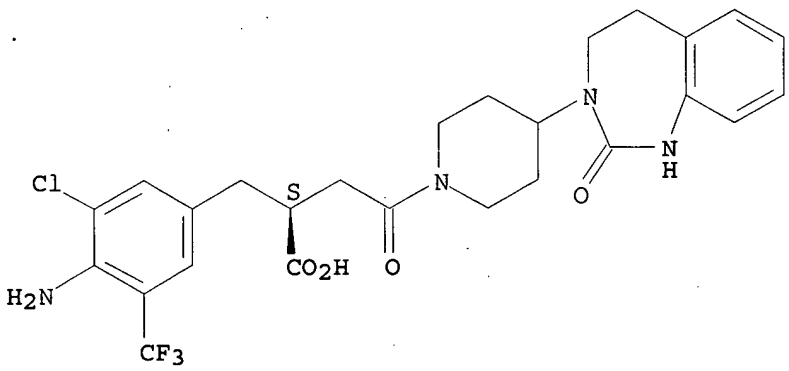
RN 688019-10-5 HCAPLUS
CN 1-Piperidinebutanamide, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-N-[[3-(aminomethyl)phenyl]methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

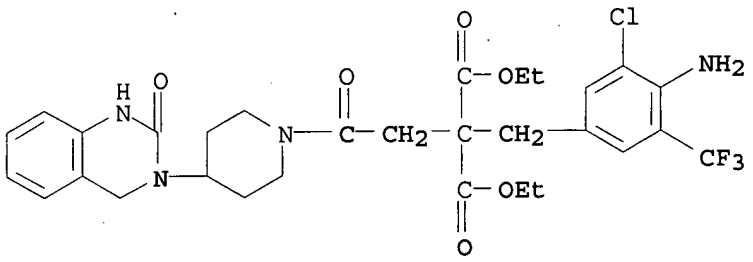


IT 688020-76-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzo-1,3-diazepin-2-ones and related compds. as CGRP receptor antagonists for the treatment of migraine headaches)
RN 688020-76-0 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI) (CA INDEX NAME)

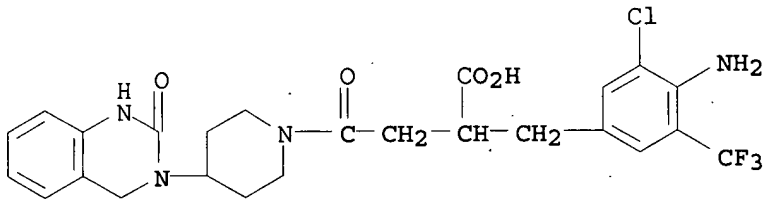
Absolute stereochemistry.



IT 688020-58-8P 688020-59-9P 688020-74-8P
688020-75-9P 688020-82-8P 688020-84-0P
688020-85-1P 688020-86-2P 688020-87-3P
688020-88-4P 688020-89-5P 688020-90-8P
688020-94-2P 688020-95-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzo-1,3-diazepin-2-ones and related compds. as CGRP receptor antagonists for the treatment of migraine headaches)
RN 688020-58-8 HCAPLUS
CN Propanedioic acid, [[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl][2-[4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-1-piperidinyl]-2-oxoethyl]-, diethyl ester (9CI) (CA INDEX NAME)

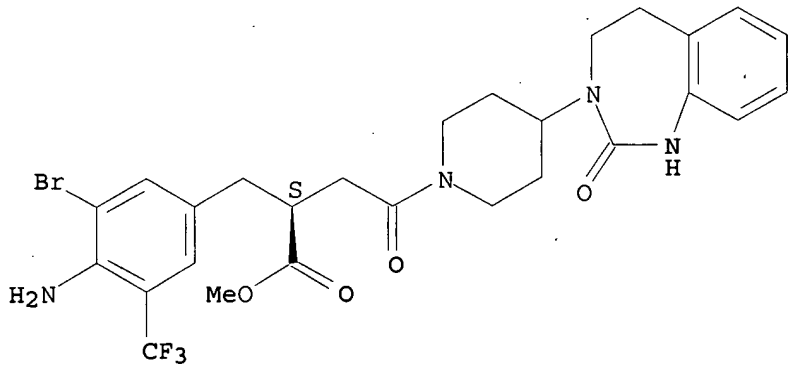


RN 688020-59-9 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-γ-oxo- (9CI) (CA INDEX NAME)



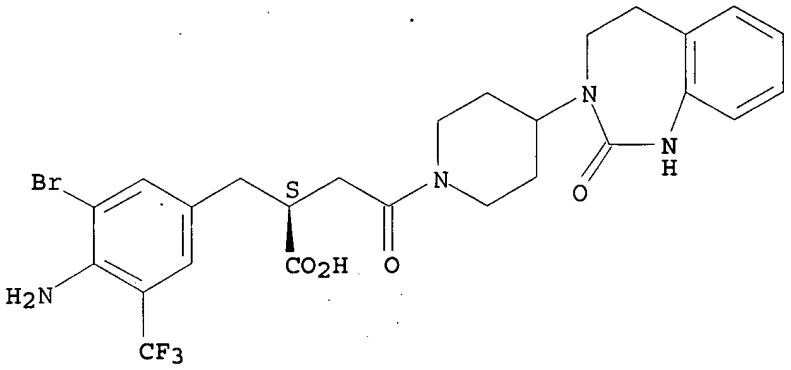
RN 688020-74-8 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-bromo-5-(trifluoromethyl)phenyl]methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



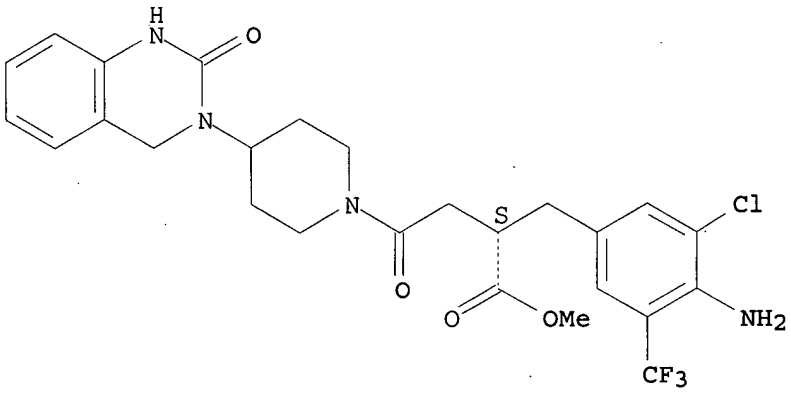
RN 688020-75-9 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-bromo-5-(trifluoromethyl)phenyl]methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



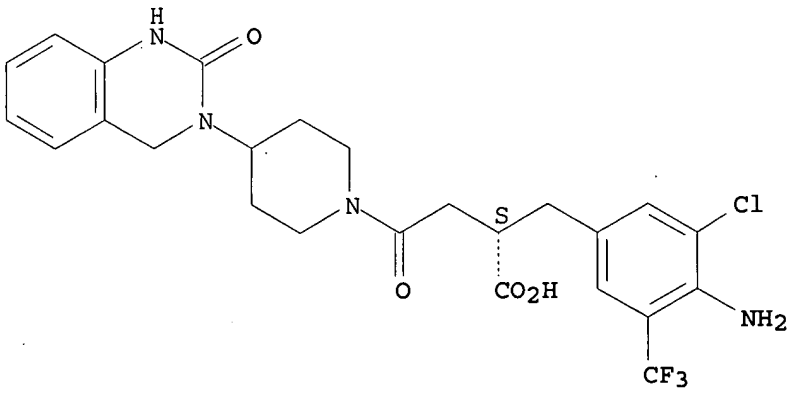
RN 688020-82-8 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-γ-oxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 688020-84-0 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-γ-oxo-, (αS)- (9CI) (CA INDEX NAME)

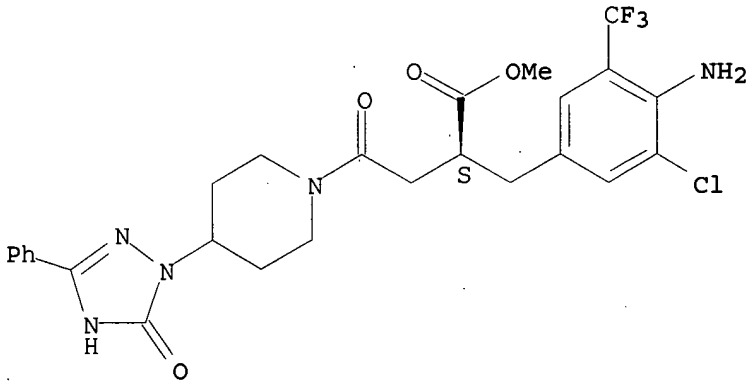
Absolute stereochemistry.



RN 688020-85-1 HCAPLUS

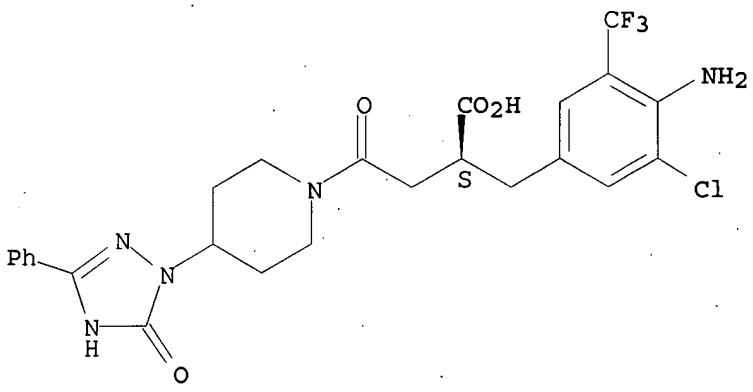
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(2,5-dihydro-5-oxo-3-phenyl-1H-1,2,4-triazol-1-yl)-γ-oxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



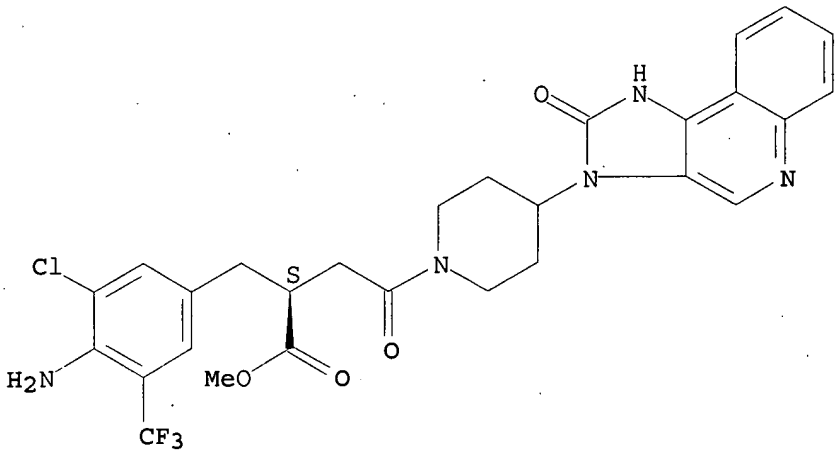
RN 688020-86-2 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(2,5-dihydro-5-oxo-3-phenyl-1H-1,2,4-triazol-1-yl)-γ-oxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



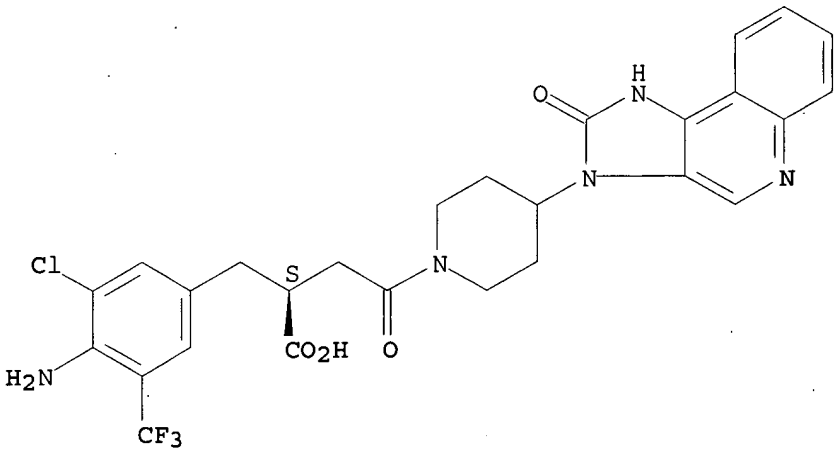
RN 688020-87-3 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,2-dihydro-2-oxo-3H-imidazo[4,5-c]quinolin-3-yl)-γ-oxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



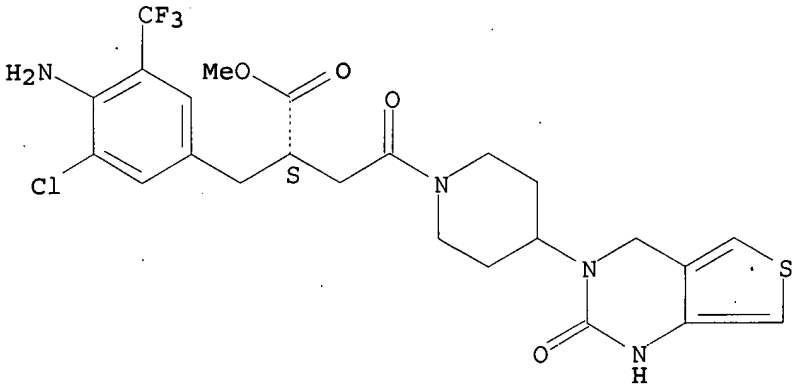
RN 688020-88-4 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,2-dihydro-2-oxo-3H-imidazo[4,5-c]quinolin-3-yl)-γ-oxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



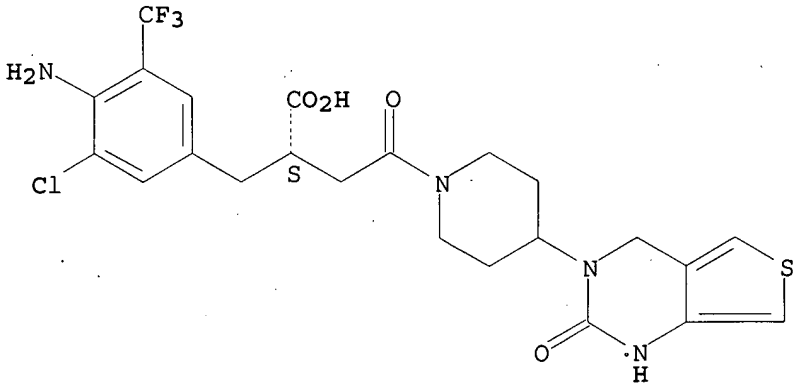
RN 688020-89-5 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,2-dihydro-2-oxothieno[3,4-d]pyrimidin-3(4H)-yl)-γ-oxo-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



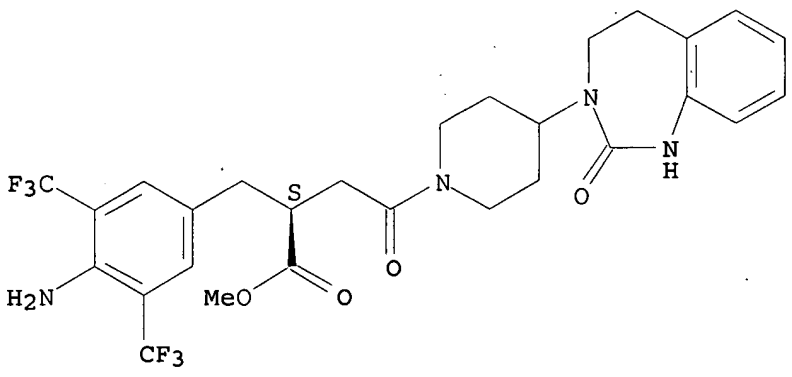
RN 688020-90-8 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-4-(1,2-dihydro-2-oxothieno[3,4-d]pyrimidin-3(4H)-yl)-γ-oxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



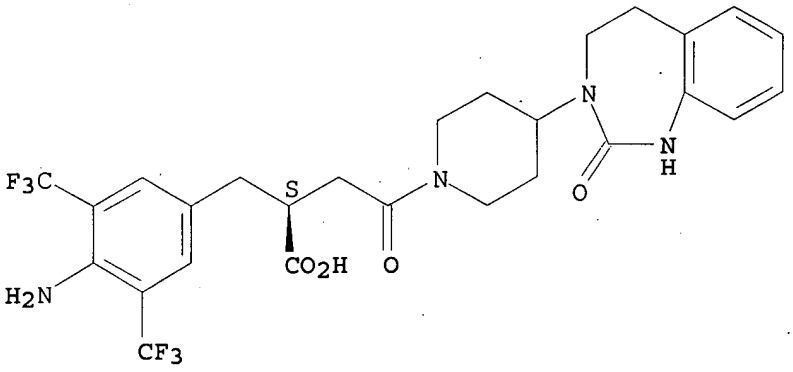
RN 688020-94-2 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3,5-bis(trifluoromethyl)phenyl]methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, methyl ester, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 688020-95-3 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3,5-bis(trifluoromethyl)phenyl]methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

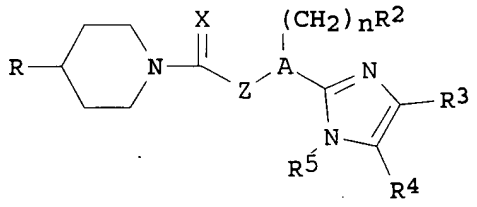
L4 ANSWER 5 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:737751 HCAPLUS
DOCUMENT NUMBER: 139:261330
TITLE: Preparation of benzodiazepine-substituted piperidines for use in treating cardiovascular diseases
INVENTOR(S): Hurnaus, Rudolf; Rudolf, Klaus; Mueller, Stephan Georg; Stenkamp, Dirk; Lustenberger, Philipp; Dreyer, Alexander; Gerlach, Kai; Schindler, Marcus; Arndt, Kirsten; Bauer, Eckhart
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma Gmbh & Co. Kg, Germany; et al.
SOURCE: PCT Int. Appl., 200 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076432	A1	20030918	WO 2003-EP2417	20030310
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10211770	A1	20031002	DE 2002-10211770	20020314
CA 2476031	AA	20030918	CA 2003-2476031	20030310
AU 2003212323	A1	20030922	AU 2003-212323	20030310
EP 1487821	A1	20041222	EP 2003-708202	20030310
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

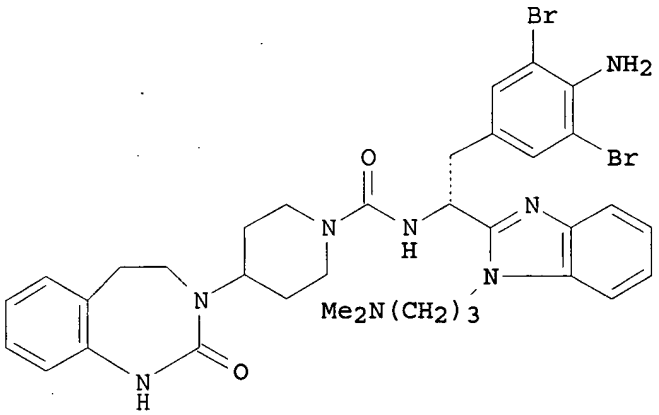
JP 2005527519	T2	20050915	JP 2003-574649		20030310
US 2003236282	A1	20031225	US 2003-388273		20030313
US 7026312	B2	20060411			
US 2005215546	A1	20050929	US 2005-138868		20050526
PRIORITY APPLN. INFO.:			DE 2002-10211770	A	20020314
			US 2002-396660P	P	20020717
			WO 2003-EP2417	W	20030310
			US 2003-388273	A1	20030313

OTHER SOURCE(S): MARPAT 139:261330

GI



I



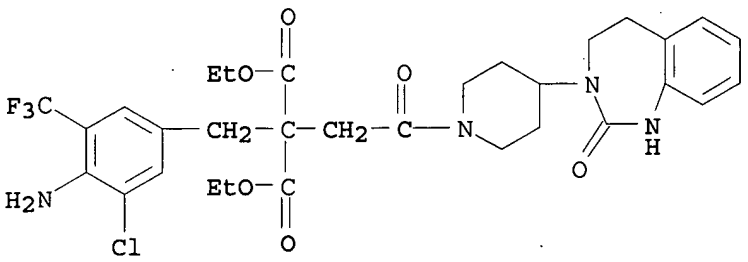
II

AB Title compds. I [R = (un)substituted 5-7-membered aza-, diaza-, triaza-oxaaza- thiaza- thiadiaza-heterocycle; X = O, (un)substituted NH, :NCN, :NSO2R1; Z = (un)substituted CH2, NH; A = (un)substituted CH; n = 1, 2; R1 = alkyl, (un)substituted Ph; R2 = substituted Ph; R3, R4 = H, (un)substituted alkyl, Ph, naphthyl, heterocyclic; R5 = H, (un)substituted alkyl, OH, naphthyl, heteroaryl, cycloalkyl] were prepared for use as CGRP antagonists (no data). Thus, the title compound II was prepared by cyclizing the benzodiazepinylpiperidinylcarbonylaminopropionic acid fragment with 2-Me2N(CH2)3C6H4NH2 to form the benzimidazole moiety.

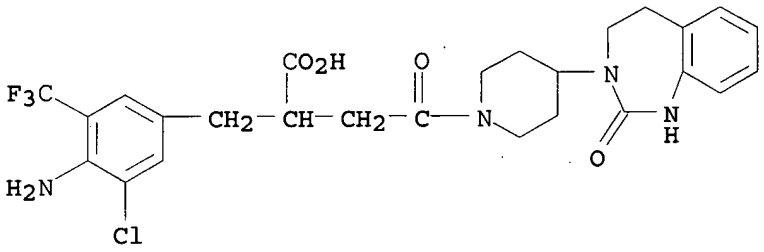
IT 600725-57-3P 600725-58-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzodiazepine-substituted piperidines for use in treating cardiovascular diseases)

RN 600725-57-3 HCAPLUS

CN Propanedioic acid, [[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl][2-oxo-2-[4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)-1-piperidinyl]ethyl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 600725-58-4 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[[4-amino-3-chloro-5-(trifluoromethyl)phenyl]methyl]-γ-oxo-4-(1,2,4,5-tetrahydro-2-oxo-3H-1,3-benzodiazepin-3-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:97391 HCAPLUS
DOCUMENT NUMBER: 138:137324
TITLE: Preparation of phenylpropionic acid derivatives as α4 integrin inhibitors
INVENTOR(S): Chiba, Akira; Sagi, Kazuyuki; Yoshimura, Toshihiko; Okuzumi, Tatsuya; Izawa, Hiroyuki; Murata, Masahiro
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003010135	A1	20030206	WO 2002-JP7543	20020725
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004236147	A1	20041125	US 2004-763237	20040126
PRIORITY APPLN. INFO.:			JP 2001-225749 A	20010726

WO 2002-JP7543 A1 20020725

OTHER SOURCE(S): MARPAT 138:137324
GI

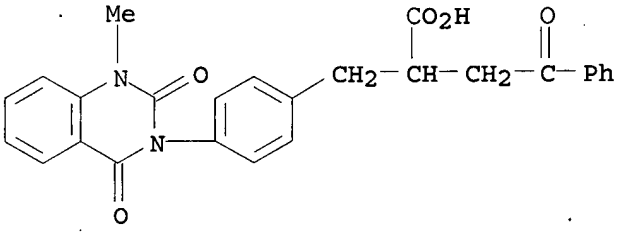
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Phenylpropionic acid derivs. represented by the general formula (I) [wherein A = Q-Q4, (un)substituted Ph, NR1-Z, NR1-CO-Z, NR1-SO2-Z, NR1-CONH-Z, NR1-C(:S)-NH-Z; wherein Z = (un)substituted Ph, lower alkyl, lower alkenyl, lower alkynyl, cycloalkyl, cycloalkyl-lower alkyl, cycloalkyl-lower alkenyl, or cycloalkyl-lower alkynyl optionally containing a heteroatoms in the cycloalkyl ring, aryl, heteroaryl, cycloalkyl, etc.; R10-R17, R21, R22, R24, R25 = H, halo, OH, lower alkyl, lower alkenyl, lower alkynyl, cycloalkyl, cycloalkyl-lower alkyl, cycloalkyl-lower alkenyl, or cycloalkyl-lower alkynyl optionally containing a heteroatoms in the cycloalkyl ring, aryl, heteroaryl, aryl-lower alkyl, heteroaryl-lower alkyl, lower alkoxy, etc.; the ring Arm = benzene ring, cycloalkyl or aromatic ring containing 0, 1, 2,3, or 4 heteroatom(s) selected from O, S, and N;
R9, R20, R23 = O, (un)substituted NH, S; R18, R19 = H, lower alkyl, lower alkenyl, lower alkynyl, aryl, heteroaryl, aryl-lower alkyl, cycloalkyl, cycloalkyl-lower alkyl, cycloalkyl-lower alkenyl, or cycloalkyl-lower alkynyl optionally containing a heteroatoms in the cycloalkyl ring, etc.; B = HO, alkoxy, hydroxyl NH2, lower alkylamino; D = each (un)substituted lower alkyl, cycloalkylaryl optionally containing a heteroatoms in the ring, aryl, or heteroaryl; E = CO, CHOH; G-G1 = CH-CH2, C:CH; J, J1 = H, halo, lower alkyl, lower alkoxy, NO2] are prepared These derivs. exhibit α4 integrin inhibiting activity and are useful as therapeutic or preventive agents for various diseases in which α4 integrin participates, e.g., inflammatory diseases in which integrin-dependent adhesion participates. The above diseases include rheumatoid arthritis, inflammatory bowel diseases, systemic lupus erythematosus, multiple sclerosis, Sjoegren's syndrome, asthma, psoriasis, allergy, diabetes, cardiovascular diseases, arteriosclerosis, restenosis, tumor proliferation, tumor metastasis, and transplant rejection. Thus, cyclization of 4-oxo-4-phenylbutanoic acid in Ac2O at 90° gave 43% 5-phenyl-2,3-dihydrofuran-2-one which underwent condensation with 4-nitrobenzaldehyde in the presence of NaOAc in Ac2O at 80° for 1 h to give 93% 3-(4-nitrobenzylidene)-5-phenyl-2,3-dihydrofuran-2-one (II). Ring-opening methanolysis of II with NaOMe in MeOH gave 84% 2-(4-nitrobenzylidene)-4-oxo-4-phenylbutanoic acid Me ester which was hydrogenated over 7.5% Pd/C in ethanol to give 28% 2-(4-aminobenzyl)-4-oxo-4-phenylbutanoic acid Me ester (III). Cyclocondensation of III with 2-isocyanatobenzoic acid Me ester in MeCN at 70° for 2 h and then at 70° for 11 h in the presence of Et3N gave 80% 2-[4-(2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxo-4-phenylbutanoic acid Me ester (IV; R = X = H, R24 = Me) which was methylated by MeI in the presence of K2CO3 in DMF for 1 h to quant. give IV (R = R24 = Me, X = H). Saponification of the latter compound with aqueous LiOH in aqueous MeOH followed by acidification with 1 N aqueous HCl gave 54% IV (R = Me, R24 = X = H). IV (R = Me, R24 = X = H) and IV (R = Me, R24 = H, X = Cl) in vitro inhibited the binding of vascular cellular adhesion mol.-1 (VCAM-1) to human B cell lymphoma cell expressing integrin α4β7 with IC50 of ≤20 to <100 μmol/L and ≤0.9 μmol/L, resp.

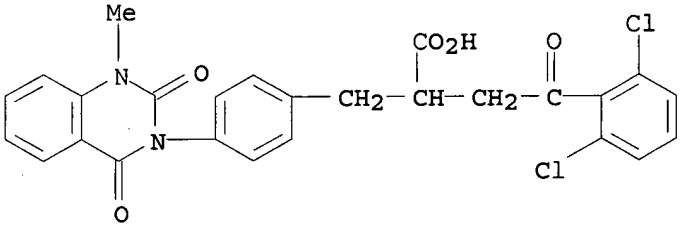
IT 493004-39-0P, 4-Phenyl-2-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxobutanoic acid 493004-40-3P, 4-(2,6-Dichlorophenyl)-2-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxobutanoic acid 493004-41-4P

, 4-(2,6-Difluorophenyl)-2-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxobutanoic acid 493004-42-5P , 4-(4-Chlorophenyl)-2-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxobutanoic acid 493004-44-7P, 4-(2,6-Dichlorophenyl)-2-[4-[[[(2-methoxycarbonylphenyl)amino]carbonyl]amino]benzyl]-4-oxobutanoic acid 493004-45-8P, 4-(2,6-Dichlorophenyl)-4-hydroxy-2-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]butanoic acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of phenylpropionic acid derivs. as α4 integrin inhibitors for prevention or treatment of α4 integrin-participating various diseases)

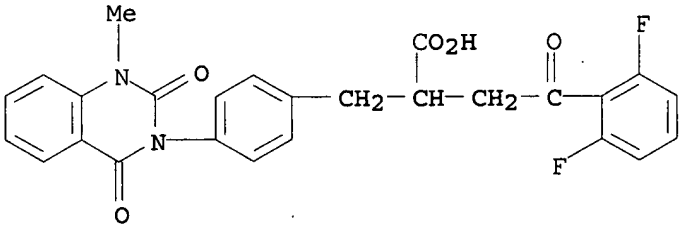
RN 493004-39-0 HCAPLUS
CN Benzenebutanoic acid, α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo- (9CI) (CA INDEX NAME)



RN 493004-40-3 HCAPLUS
CN Benzenebutanoic acid, 2,6-dichloro-α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo- (9CI) (CA INDEX NAME)

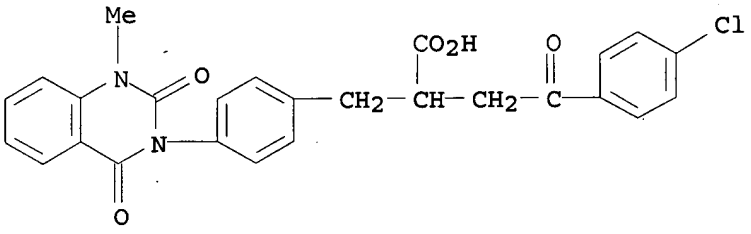


RN 493004-41-4 HCAPLUS
CN Benzenebutanoic acid, α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-2,6-difluoro-γ-oxo- (9CI) (CA INDEX NAME)

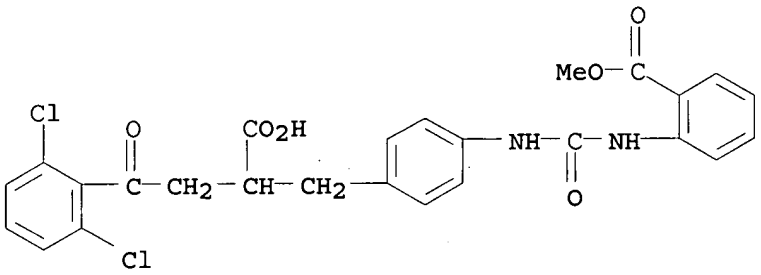


RN 493004-42-5 HCAPLUS

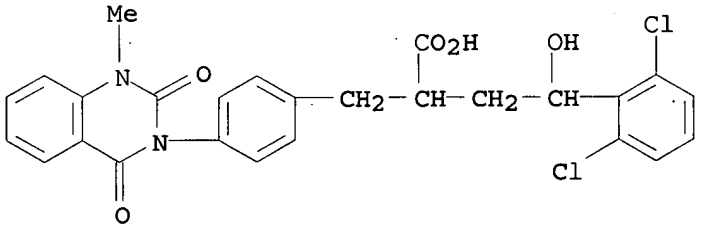
CN Benzenebutanoic acid, 4-chloro-α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo- (9CI) (CA INDEX NAME)



RN 493004-44-7 HCAPLUS
CN Benzenebutanoic acid, 2,6-dichloro-α-[[4-[[[[2-(methoxycarbonyl)phenyl]amino]carbonyl]amino]phenyl]methyl]-γ-oxo- (9CI) (CA INDEX NAME)



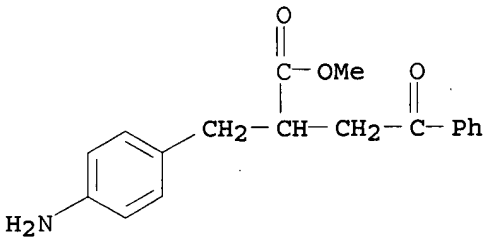
RN 493004-45-8 HCAPLUS
CN Benzenebutanoic acid, 2,6-dichloro-α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-hydroxy- (9CI) (CA INDEX NAME)



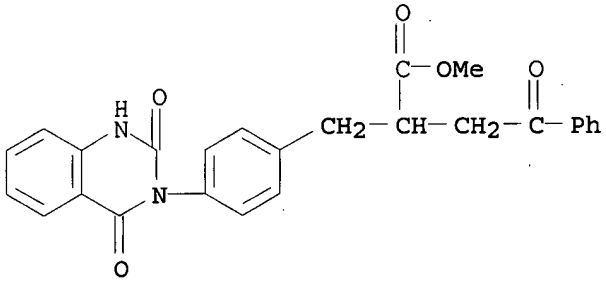
IT 493004-47-0P, 2-(4-Aminobenzyl)-4-oxo-4-phenylbutanoic acid methyl ester 493004-48-1P, 2-[4-(2,4-Dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxo-4-phenylbutanoic acid methyl ester 493004-49-2P, 2-[4-(1-Methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxo-4-phenylbutanoic acid methyl ester 493004-57-2P, 4-(2,6-Dichlorophenyl)-2-[4-(1-methyl-2,4-dioxo-1,2,3,4-tetrahydroquinazolin-3-yl)benzyl]-4-oxobutanoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of phenylpropionic acid derivs. as α4 integrin inhibitors for prevention or treatment of α4 integrin-participating various diseases)

RN 493004-47-0 HCAPLUS
CN Benzenebutanoic acid, α-[(4-aminophenyl)methyl]-γ-oxo-, methyl

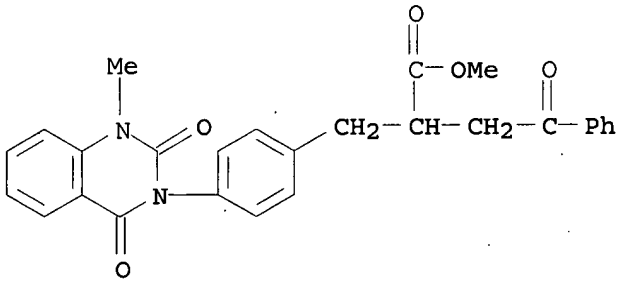
ester (9CI) (CA INDEX NAME)



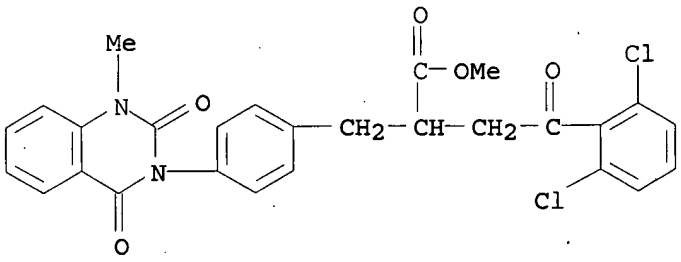
RN 493004-48-1 HCAPLUS
CN Benzenebutanoic acid, α-[[4-(1,4-dihydro-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo-, methyl ester (9CI) (CA INDEX NAME)



RN 493004-49-2 HCAPLUS
CN Benzenebutanoic acid, α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo-, methyl ester (9CI) (CA INDEX NAME)



RN 493004-57-2 HCAPLUS
CN Benzenebutanoic acid, 2,6-dichloro-α-[[4-(1,4-dihydro-1-methyl-2,4-dioxo-3(2H)-quinazolinyl)phenyl]methyl]-γ-oxo-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

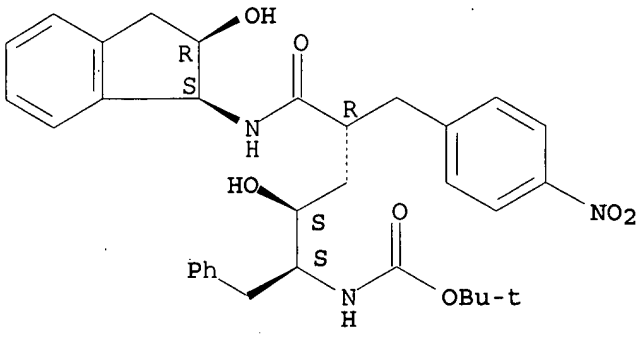
L4 ANSWER 7 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:49282 HCAPLUS
DOCUMENT NUMBER: 139:159421
TITLE: A priori molecular descriptors in QSAR: a case of HIV-1 protease inhibitors I. The chemometric approach
AUTHOR(S): Kiralj, Rudolf; Ferreira, Marcia M. C.
CORPORATE SOURCE: Instituto de Quimica, Universidade Estadual de Campinas, Campinas, 13083-970, Brazil
SOURCE: Journal of Molecular Graphics & Modelling (2003), 21(5), 435-448
CODEN: JMGMFI; ISSN: 1093-3263
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A quant. structure-activity relationship (QSAR) study on 48 peptidic HIV-1 protease inhibitors was performed. Fourteen a priori mol. descriptors were used to build QSAR models. Hierarchical cluster anal. (HCA), principal component anal. (PCA) and partial least squares (PLS) regression were employed. PLS models with 32/16 (model I) and 48/0 (model II) mols. in the training/external validation set were constructed. The a priori mol. descriptors were related to two energetic variables using PLS. HCA and PCA on data from model II classified the inhibitors as slightly, moderately and highly active; three principal components, the chemical nature of which has been highlighted, are enough to describe the enzyme-inhibitor binding. Model I (r2 = 0.91, q2 = 0.84) is comparable to literature models obtained by various QSAR softwares, which justified the use of a priori descriptors.

IT 126410-15-9 126410-17-1
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(priori mol. descriptors in QSAR and a case of HIV-1 protease inhibitors with the chemometric approach)

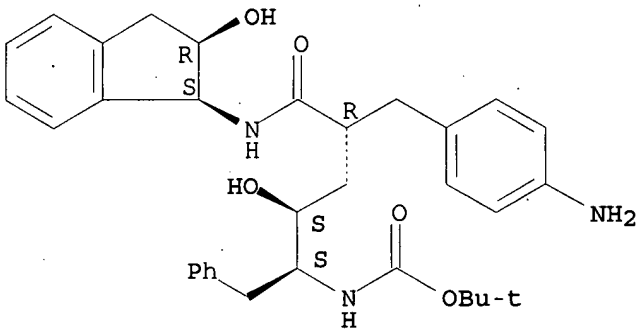
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



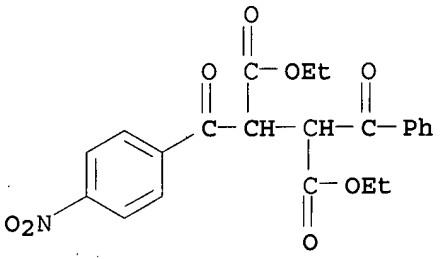
RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:881498 HCAPLUS
DOCUMENT NUMBER: 139:245816
TITLE: Product class 9: furans
AUTHOR(S): Koenig, B.
CORPORATE SOURCE: Institut fuer Organische Chemie, Universitaet Regensburg, Regensburg, 93053, Germany
SOURCE: Science of Synthesis (2002), 9, 183-285
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review on the preparation of furan derivs. via ring transformations (e.g., ring opening), cyclization, aromatization and substituent modification.
IT 600162-22-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of furans via cyclization, ring transformations, aromatization and substituent modification)
RN 600162-22-9 HCAPLUS
CN Butanedioic acid, 2-benzoyl-3-(4-nitrobenzoyl)-, diethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 737 THERE ARE 737 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

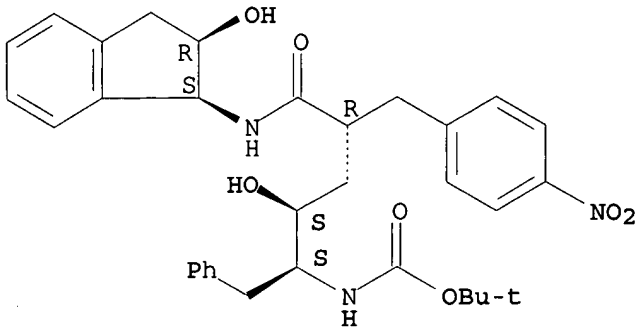
L4 ANSWER 9 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:116436 HCAPLUS
DOCUMENT NUMBER: 136:303571
TITLE: E-State Modeling of HIV-1 Protease Inhibitor Binding Independent of 3D Information
AUTHOR(S): Maw, Hlaing Hlaing; Hall, Lowell H.
CORPORATE SOURCE: Department of Chemistry, Eastern Nazarene College, Quincy, MA, 02170, USA
SOURCE: Journal of Chemical Information and Computer Sciences (2002), 42(2), 290-298
CODEN: JCISD8; ISSN: 0095-2338
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Data for HIV-1 protease inhibitors (in vitro enzyme binding) were used as a training set to develop a QSAR model based on topol. descriptors, including two hydrogen E-state indexes, along with a mol. connectivity χ and a κ shape index. A statistically satisfactory four-variable model was obtained for the 32 compds. in the training set, r2 = 0.86, s = 0.60, and q2 = 0.79, without the use of information from 3D geometries or detailed interaction energy calcns. The model was validated through the prediction of 15 compds. in the external test set, yielding a mean absolute error, MAE, = 0.82. Structure interpretation is given for each variable to assist in the design of new compds. Structure features emphasized in the model include hydrogen bond donating ability, nonpolar groups, skeletal branching, and mol. globularity. On the basis of these statistical criteria, this E-state model may be considered useful for prediction of pIC50 values for new HIV-1 protease inhibitors.

IT 126410-15-9 126410-17-1
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(E-state modeling of HIV-1 protease inhibitor binding independent of 3D information)

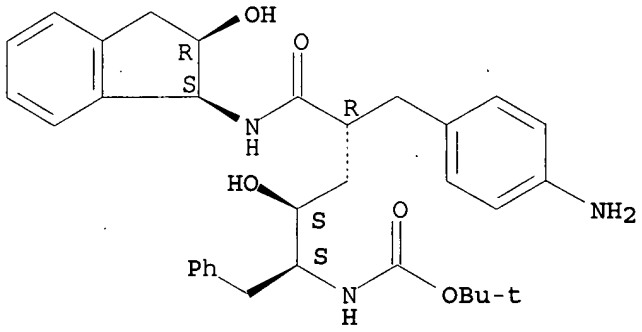
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

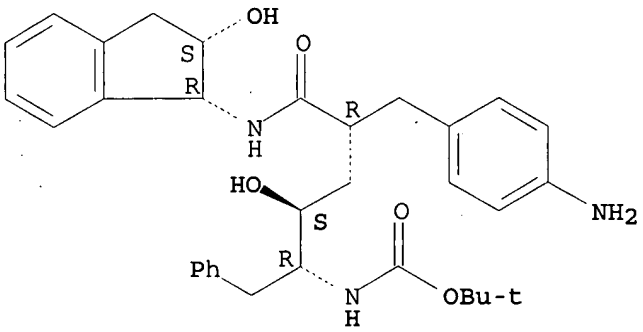
L4 ANSWER 10 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:720732 HCAPLUS
DOCUMENT NUMBER: 134:36677
TITLE: Computational Studies on HIV-1 Protease Inhibitors: Influence of Calculated Inhibitor-Enzyme Binding Affinities on the Statistical Quality of 3D-QSAR CoMFA Models
AUTHOR(S): Jayatilleke, Philippa R. N.; Nair, Anil C.; Zauhar, Randy; Welsh, William J.
CORPORATE SOURCE: Department of Chemistry and Center for Molecular Electronics, University of Missouri-St. Louis, St. Louis, MO, 63121, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(23), 4446-4451
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A theor. study was performed on a set of 38 human immunodeficiency type 1 (HIV-1) protease inhibitors that are structurally similar to the AIDS drug Indinavir. Comparison between the computed binding energies and exptl. activity data (pIC50) found a high degree of correlation (r2 = 0.82). Three-dimensional quant. structure-activity relationship (3D-QSAR) models using comparative mol. field anal. (CoMFA) yielded predicted activities

that were in excellent agreement with the corresponding exptl. determined values. Inclusion of the calculated enzyme-inhibitor binding energy as an addnl. descriptor in the CoMFA model yielded a significant improvement in the internal predictive ability of our model (q2 = 0.45 to q2 = 0.69). Sep. CoMFA models were constructed to evaluate the influence of different alignment schemes (Atom Fit and Field Fit) and different partial atomic charge assignment schemes (Discover CVFF, Gasteiger-Marsili, and AM1-ESP) on the statistical quality of the models.

IT 312694-70-5 312694-71-6
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(computational studies on HIV-1 protease inhibitors and influence of calculated inhibitor-enzyme binding affinities on statistical quality of 3D-QSAR CoMFA models)

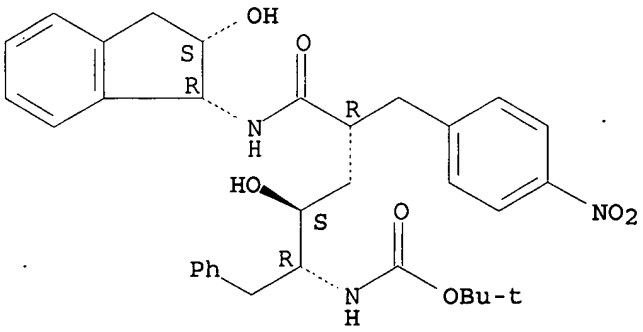
RN 312694-70-5 HCAPLUS
CN Carbamic acid, [(1R,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1R,2S)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312694-71-6 HCAPLUS
CN Carbamic acid, [(1R,2S,4R)-5-[[(1R,2S)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

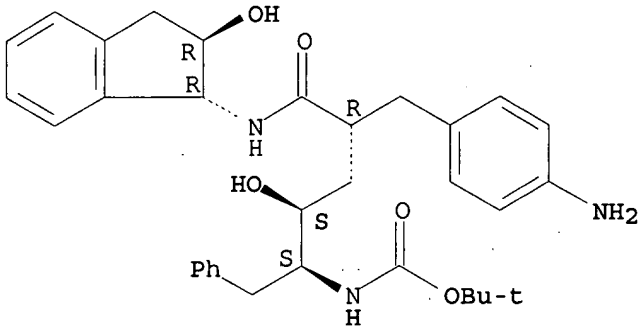
L4 ANSWER 11 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:500184 HCAPLUS

DOCUMENT NUMBER: 133:234344
TITLE: DoMCoSAR: A Novel Approach for Establishing the Docking Mode That Is Consistent with the Structure-Activity Relationship. Application to HIV-1 Protease Inhibitors and VEGF Receptor Tyrosine Kinase Inhibitors
AUTHOR(S): Vieth, Michal; Cummins, David J.
CORPORATE SOURCE: Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN, 46285, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(16), 3020-3032
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB DoMCoSAR is a novel approach for statistically determining the docking mode that is consistent with a structure-activity relationship. The approach establishes the binding mode for the compds. in a chemical series with the assumption that all mols. exhibit the same binding mode. It involves three stages. In the first stage all mols. that belong to a given chemical series are docked to the active site of the protein target. The only bias used in the docking at this stage involves the location of the protein binding site. Coordinates of the common substructure (CS) that results from the unbiased docking are then clustered to establish the major substructure docking modes. In the second stage all mols. are docked to the major docking modes (MDMs) with constraints based on the common substructure. The third stage generates, for the major docking modes, interaction-based descriptors that include electrostatic, VDW, strain, and solvation contributions. The problem of docking mode evaluation is now reduced to the question of which descriptor set is more predictive. To establish a quant. comparison of the descriptor sets associated with the major docking modes, we use 50 instances of random 4-fold cross-validation. For each 4-fold cross-validation the predictive squared correlation coefficient (R2) is computed. T-Tests are applied to establish significance of the differences in mean R for one docking mode vs. another. We test the methodol. on two test cases: HIV-1 protease inhibitors (Holloway et al. J. Med. Chemical 1995, 38, 305-317) and vascular endothelial growth factor (VEGF) receptor tyrosine kinase oxoindoles (Sun et al. J. Med. Chemical 1998, 41, 2588-2603). For both test cases there is statistically significant preference for the binding mode consistent with the x-ray structure. The appeal of this methodol. is that researchers gain the objectivity of statistical justification for the selected docking mode. The methodol. is relatively insensitive to subtle variations of the protein structure that include, but are not limited to, side chain and small backbone rearrangement during binding. In addition, predictive models that result from the approach can be used to further optimize chemical series.

IT 293301-86-7 293301-88-9
RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(HIV-1 protease-inhibitor; DoMCoSAR - novel approach for establishing docking mode that is consistent with structure-activity relationship with application to HIV-1 protease inhibitors and VEGF receptor tyrosine kinase inhibitors)

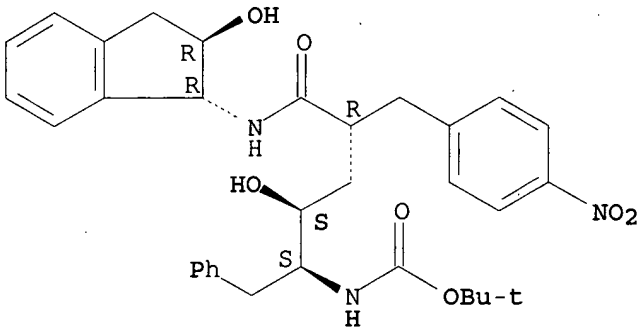
RN 293301-86-7 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1R,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 293301-88-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1R,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

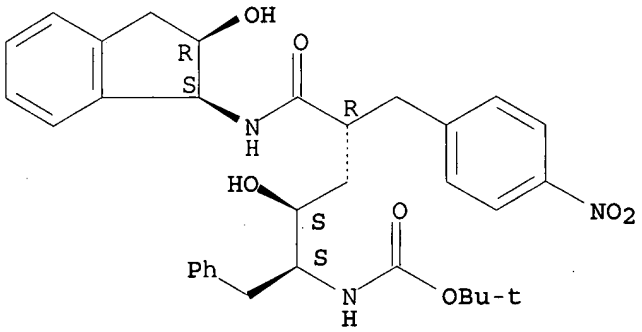
L4 ANSWER 12 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:82352 HCAPLUS
DOCUMENT NUMBER: 132:231512
TITLE: A novel hydropathic intermolecular field analysis (HIFA) for the prediction of ligand-receptor binding affinities
AUTHOR(S): Semus, Simon F.
CORPORATE SOURCE: Department of Biological Chemistry, Wyeth-Ayerst Research, Princeton, NJ, 08543, USA
SOURCE: Medicinal Chemistry Research (1999), 9(7/8), 535-547
CODEN: MCREEB; ISSN: 1054-2523
PUBLISHER: Birkhaeuser Boston
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A novel method is described for the evaluation of ligand-receptor binding affinities using a grid based 3D QSAR approach. The anal. utilizes HINT calculated hydropathic fields that more accurately reflect the interaction between a ligand and a receptor than the probe atom method implemented in CoMFA. This method has been applied to a series of HIV protease inhibitors and found to produce a much superior predictive model. The HINT hydropathic intermol. field anal. (HIFA) method described herein represents the first 3D QSAR method that truly quantifies the interaction between ligand and receptor.

IT 126410-15-9 126410-17-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(novel hydropathic intermol. field anal. (HIFA) for prediction of ligand-receptor binding affinities of HIV1 protease inhibitors)

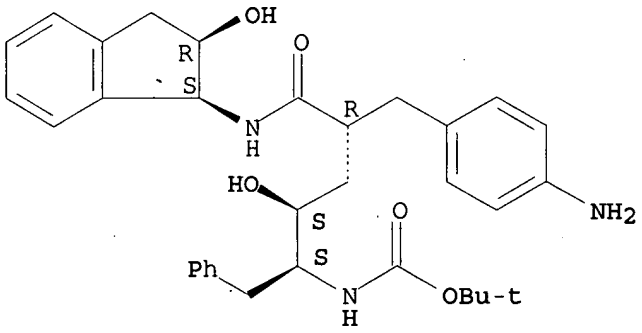
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:529580 HCAPLUS
DOCUMENT NUMBER: 131:223019
TITLE: GA strategy for variable selection in QSAR studies. Enhancement of comparative molecular binding energy analysis by GA-based PLS method
AUTHOR(S): Hasegawa, Kiyoshi; Kimura, Toshiro; Funatsu, Kimito
CORPORATE SOURCE: Tokyo Research Laboratories, Kowa Co. Ltd., Higashimurayama, 189, Japan
SOURCE: Quantitative Structure-Activity Relationships (1999), 18(3), 262-272

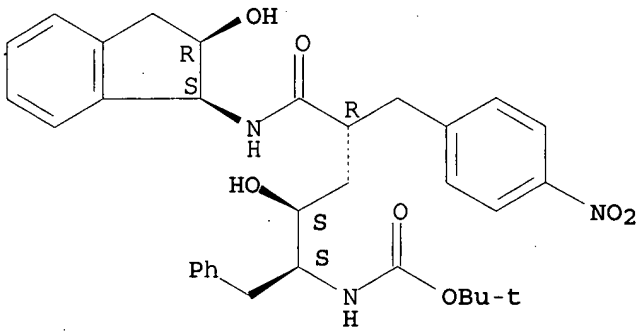
CODEN: QSARDI; ISSN: 0931-8771
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A study was performed to examine whether genetic algorithm-based partial least squares (GAPLS) developed for variable selection can enhance prediction and interpretation of the comparative mol. binding energy (COMBINE) model. Structure-activity data of inhibitors of HIV-1 protease were used as a test example. By applying GAPLS to this data set, several improved PLS models with a high cross-validated r2 value and low number of variables were obtained. To select a best model from them, external validation was performed for each model. The finally selected model was further examined by comparing with the 3D structure of HIV-1 protease in computer graphics and its agreement was confirmed.

IT 126410-15-9 126410-17-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitory activity on HIV-1 protease by genetic algorithm-based partial least squares method)

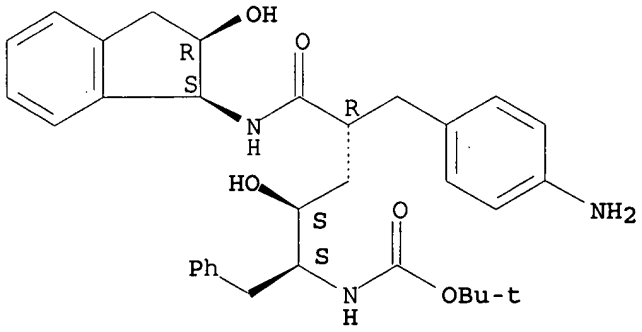
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

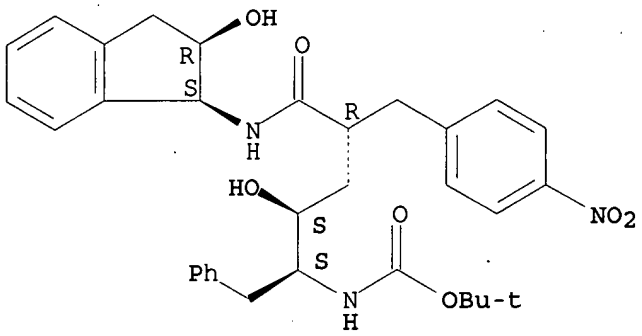
L4 ANSWER 14 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:518774 HCAPLUS
DOCUMENT NUMBER: 129:239460
TITLE: Simulation of alternative binding modes in a structure-based QSAR study of HIV-1 protease inhibitors
AUTHOR(S): Pastor, Manuel; Perez, Carlos; Gago, Federico
CORPORATE SOURCE: Department of Pharmacology, University of Alcala, Alcala de Henares, E-28871, Spain
SOURCE: Journal of Molecular Graphics & Modelling (1998), Volume Date 1997, 15(6), 364-371
CODEN: JMGMFI; ISSN: 1093-3263
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have used a published set of inhibitors of HIV-1 protease to build a COMBINE-type structure-based QSAR model with good predictive ability (r2 = 0.90, q2 = 0.69).2. Since the compds. in the training series exhibit most of their structural variability on one-half of the pseudosym. binding cavity and only one binding orientation was explored for each mol., the model describes mainly the effect of the structural changes on interactions involving only one-half of the binding cavity (pockets S1' and 2'). Thus, the model cannot be expected to give accurate predictions for new compds. exhibiting structural variation in both halves. The model does in fact show a tendency to underpredict slightly the biol. activity of the mols. in the external test set. In an attempt to improve the quality of the model, both possible orientations of the ligands are now considered so that structural variation takes place in all binding pockets. One possibility would have been to build an addnl. set of complexes with the inhibitors docked in a reversed orientation. The alternative we have explored, however, consists of manipulating the data matrix describing the interaction energies so that each row is duplicated and the order of the variables in the duplicated rows is swapped between subunits. This simple approach has produced a new model that is similar in quality to the original model (r2 = 0.89, q2 = 0.64) but lacks the tendency to underpredict the activity of the compds. in the external set. Moreover, since equivalent residues are assigned equivalent wts., the model is insensitive to ligand orientation and is easier to interpret.

IT 126410-15-9 126410-17-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(simulation of alternative binding modes in a structure-based QSAR study of HIV-1 protease inhibitors)

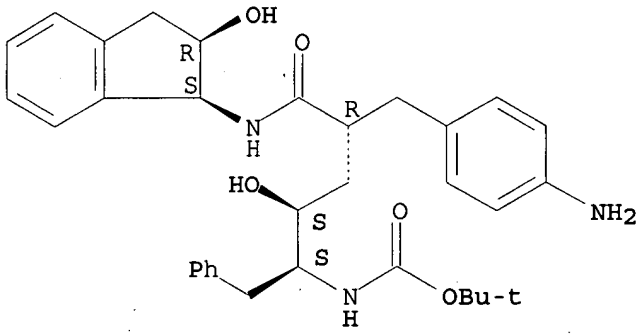
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:197358 HCAPLUS
DOCUMENT NUMBER: 128:257695
TITLE: Preparation of modified amino acids and their use as calcitonin gene-related peptide antagonists in pharmaceutical compositions
INVENTOR(S): Rudolf, Klaus; Eberlein, Wolfgang; Engel, Wolfhard; Pieper, Helmut; Doods, Henri; Hallermayer, Gerhard; Entzeroth, Michael; Wienen, Wolfgang
PATENT ASSIGNEE(S): Karl Thomae G.m.b.H., Germany
SOURCE: PCT Int. Appl., 461 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

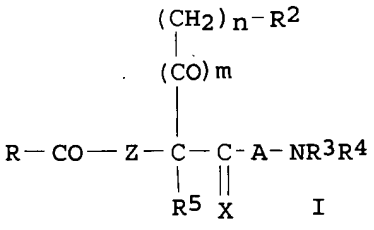
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9811128	A1	19980319	WO 1997-EP4862	19970908
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG,				

	US, UZ, VN, YU, ZW				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
DE	19636623	A1	19980312	DE 1996-19636623	19960910
DE	19720011	A1	19981119	DE 1997-19720011	19970514
CA	2262818	AA	19980319	CA 1997-2262818	19970908
AU	9741196	A1	19980402	AU 1997-41196	19970908
AU	721035	B2	20000622		
EP	927192	A1	19990707	EP 1997-938928	19970908
EP	927192	B1	20040512		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR	9712023	A	19990831	BR 1997-12023	19970908
JP	2000505100	T2	20000425	JP 1998-513227	19970908
JP	3483893	B2	20040106		
AT	266673	E	20040515	AT 1997-938928	19970908
EE	4375	B1	20041015	EE 1999-115	19970908
PL	190180	B1	20051130	PL 1997-331989	19970908
NO	9901130	A	19990505	NO 1999-1130	19990309
KR	2000044040	A	20000715	KR 1999-702008	19990310
BG	64214	B1	20040531	BG 1999-103250	19990315
US	6344449	B1	20020205	US 1999-254281	19991012
HK	1021192	A1	20040430	HK 1999-105722	19991208
US	2001036946	A1	20011101	US 2001-789391	20010221
US	2003069231	A1	20030410	US 2002-119875	20020410
US	2004214819	A1	20041028	US 2004-835495	20040429

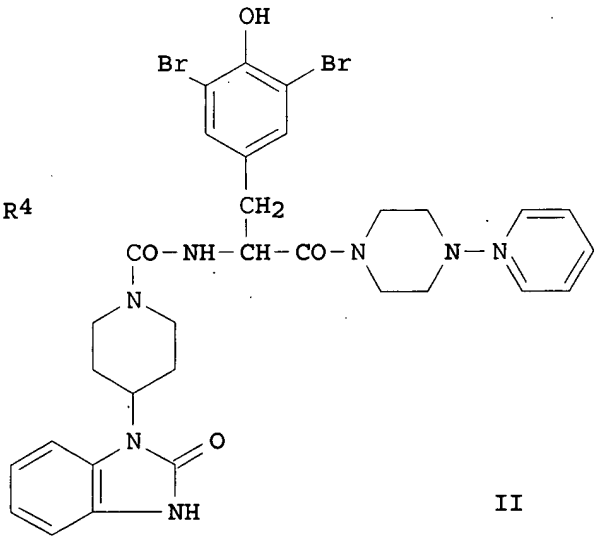
PRIORITY APPLN. INFO.:	DE 1996-19636623	A	19960910
	DE 1997-19720011	A	19970514
	WO 1997-EP4862	W	19970908
	US 1999-254281	A1	19991012
	US 2001-789391	A1	20010221
	US 2002-119875	B1	20020410

OTHER SOURCE(S): MARPAT 128:257695

GI



I



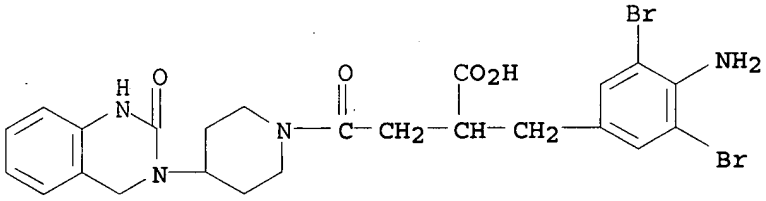
II

AB The invention concerns modified amino acids of general formula I [A =

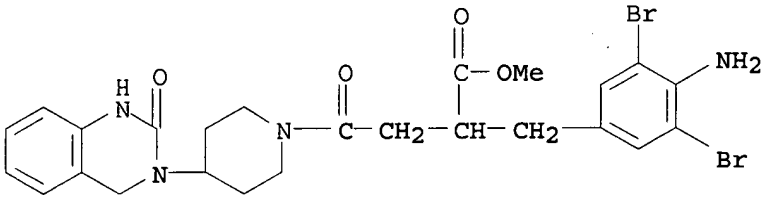
bond, CX; Z = CH2, NR1; R1 = H, alkyl, phenyl-alkyl; X = O, H,H; n = 1-2; m = 0-1; R = (substituted)alkyl; R2 = Ph, (substituted)(hetero)(bi)cycle; R3 = H, (substituted)alkyl, Ph, pyridinyl; R4 = H, (substituted)alkyl; R3R4= (hetero)cycle; R5 = H, alkyl, alkoxycarbonyl, PhCH2], pharmaceuticals containing these compds., their use and the method for their production, as well as their use for the production and purification of antibodies and as marked compds. in RIA and ELISA assays and as diagnostic or analytic auxiliary agents in neurotransmitter research. Thus, 3,5-dibromo-N2-[4-(1,3-dihydro-2(2H)-oxo-benzimidazol-1-yl)-1-piperidinyl]carbonyl-D-tyrosine was reacted with 1-(4-pyridinyl)-piperazine, to give II(22%). Title compds. show human calcitonin gene related peptide (CGRP) antagonist activity; in in-vitro binding studies with Sk-N-MC-cells, I had IC50 ≤10000 nM, and in the same system, had CGRP-antagonist activity at doses from 10-11 to 10-6 M.

IT 205060-57-7P 205060-77-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino acids and their use as calcitonin gene-related peptide antagonists in pharmaceutical compns.)

RN 205060-57-7 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[(4-amino-3,5-dibromophenyl)methyl]-4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-γ-oxo- (9CI) (CA INDEX NAME)



RN 205060-77-1 HCAPLUS
CN 1-Piperidinebutanoic acid, α-[(4-amino-3,5-dibromophenyl)methyl]-4-(1,4-dihydro-2-oxo-3(2H)-quinazolinyl)-γ-oxo-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:119593 HCAPLUS
DOCUMENT NUMBER: 128:212673
TITLE: Comparative Binding Energy Analysis of HIV-1 Protease Inhibitors: Incorporation of Solvent Effects and Validation as a Powerful Tool in Receptor-Based Drug Design
AUTHOR(S): Perez, Carlos; Pastor, Manuel; Ortiz, Angel R.; Gago, Federico
CORPORATE SOURCE: Departamento de Farmacologia, Universidad de Alcala,

E-28871, Spain
SOURCE: Journal of Medicinal Chemistry (1998), 41(6), 836-852
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

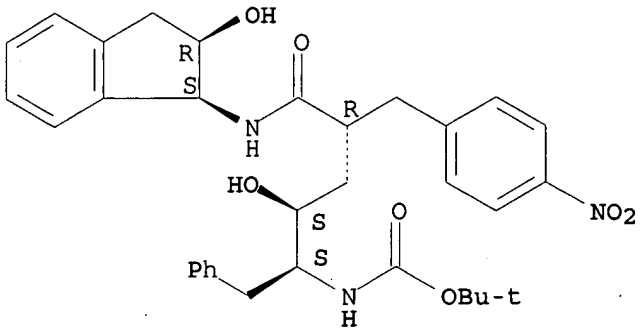
AB A comparative binding energy (COMBINE) anal. was performed on a training set of 33 HIV-1 protease inhibitors, and the resulting regression models were validated using an addnl. external set of 16 inhibitors. This data set was originally reported by Holloway et al. (1995), who showed the usefulness of mol. mechanics interaction energies for predicting the activity of novel HIV-1 protease inhibitors within the framework of the MM2X force field and linear regression techniques. The authors first used the AMBER force field on the same set of 3-dimensional structures to check up on any possible force-field dependencies. In agreement with the previous findings, the calculated raw ligand-receptor interaction energies were highly correlated with the inhibitory activities (r2 = 0.81), and the linear regression model relating both magnitudes had an acceptable predictive ability both in internal validation tests (q2 = 0.79, SDEPcv = 0.61) and when applied to the external set of 16 different inhibitors (SDEPex = 1.08). When the interaction energies were further analyzed using the COMBINE formalism, the resulting PLS model showed improved fitting properties (r2 = 0.89) and provided better estns. for the activity of the compds. in the external data set (SDEPex = 0.83). Computation of the electrostatic part of the ligand-receptor interactions by numerically solving the Poisson-Boltzmann equation did not improve the quality of the linear regression model. On the contrary, incorporation of the solvent-screened residue-based electrostatic interactions and 2 addnl. descriptors representing the electrostatic energy contributions to the partial desolvation of both the ligands and the receptor resulted in a COMBINE model that achieved a remarkable predictive ability, as assessed by both internal (q2 = 0.73, SDEPcv = 0.69) and external validation tests (SDEPex = 0.59). Finally, when all the inhibitors studied were merged into a single expanded set, a new model was obtained that explained 91% of the variance in biol. activity (r2 = 0.91), with very high predictive ability (q2 = 0.81, SDEPcv = 0.66). In addition, the COMBINE anal. provided valuable information about the relative importance of the contributions to the activity of individual residues that can be fruitfully used to design better inhibitors. All in all, COMBINE anal. is validated as a powerful methodol. for predicting binding affinities and pharmacol. activities of congeneric ligands that bind to a common receptor.

IT 126410-15-9 126410-17-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(solvent effects on comparative binding energy anal. of HIV protease inhibitors in receptor-based drug design)

RN 126410-15-9 HCAPLUS

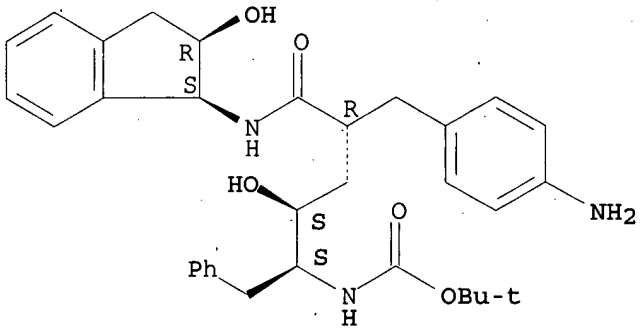
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



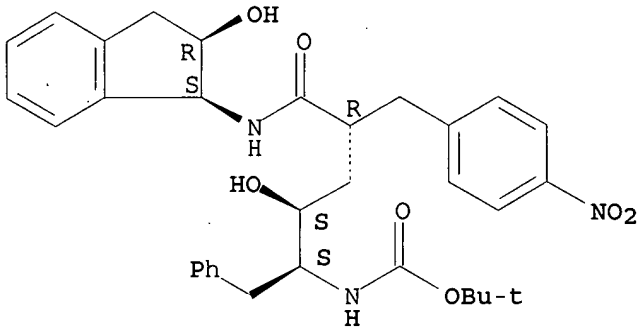
REFERENCE COUNT: 60 THERE ARE 60 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:659318 HCAPLUS
DOCUMENT NUMBER: 127:341378
TITLE: Effects of entropy on QSAR equations for HIV-1 protease: 1. Using hydropathic binding descriptors. 2. Unrestrained complex structure optimizations
AUTHOR(S): Wei, David T.; Meadows, Justin C.; Kellogg, Glen Eugene
CORPORATE SOURCE: Dep. Biomedical Eng., Sch. Eng., Virginia Commonwealth Univ., Richmond, VA, 23298-0694, USA
SOURCE: Medicinal Chemistry Research (1997), 7(4), 259-270
CODEN: MCREEB; ISSN: 1054-2523
PUBLISHER: Birkhaeuser
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The binding of HIV-1 protease inhibitors has been recently described (Holloway, M.K., et al., J. Med. Chemical 1995, 38, 305-317) in terms of a simple QSAR equation relating IC50 to a mol. mechanics energy term. The authors show that this equation can be enhanced by the addition of hydropathic binding descriptors calculated with the HINT program. Further examination of the complex structures, including unrestrained structure optimization with the Tripos Force Field in SYBYL 6.22, yield significantly poorer QSAR models for binding affinity, even with the addition of hydropathic binding terms.

IT 126410-15-9 126410-17-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(effects of entropy on QSAR equations for HIV-1 protease inhibitors using hydropathic binding descriptors and unrestrained complex structure optimizations)

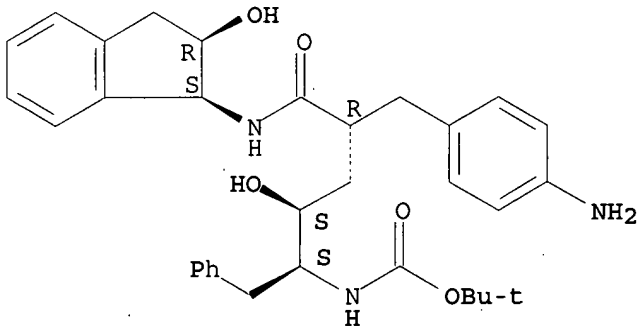
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:271492 HCAPLUS
DOCUMENT NUMBER: 125:104292
TITLE: A Priori Prediction of Activity for HIV-1 Protease Inhibitors Employing Energy Minimization in the Active Site. [Erratum to document cited in CA122:177664]
AUTHOR(S): Holloway, M. Katharine; Wai, Jenny M.; Halgren, Thomas A.; Fitzgerald, Paula M. D.; Vacca, Joseph P.; Dorsey, Bruce D.; Levin, Rhonda B.; Thompson, Wayne J.; Chen, L. Jenny; et al.
CORPORATE SOURCE: Department of Molecular Systems, Merck Research

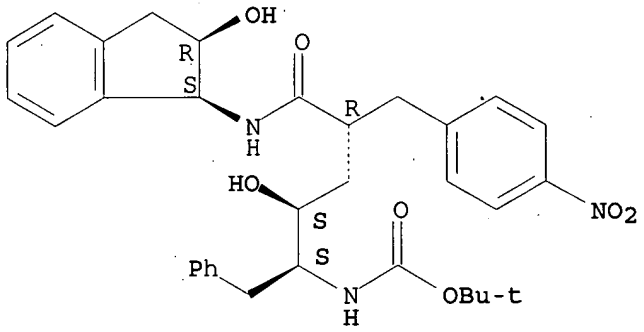
Laboratories, West Point, PA, 19486, USA
SOURCE: Journal of Medicinal Chemistry (1996), 39(11), 2280
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Equations 1-3 are corrected The errors were not reflected in the abstract or the index entries.

IT 126410-15-9 126410-17-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(energy minimization in active site for design of HIV-1 protease inhibitors (Erratum))

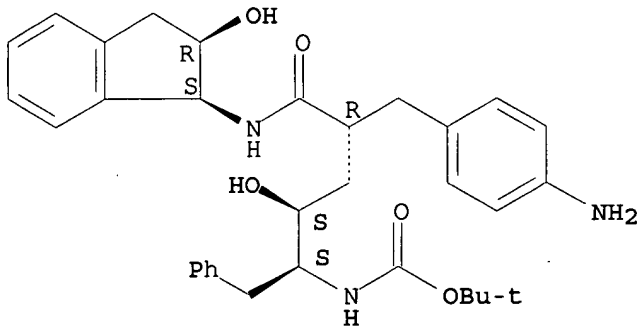
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 19 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:746789 HCAPLUS
DOCUMENT NUMBER: 123:198761
TITLE: Novel Antagonists of Platelet-Activating Factor. 1. Synthesis and Structure-Activity Relationships of

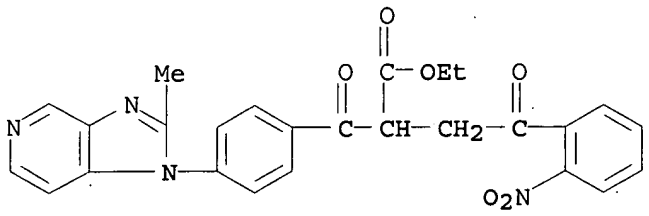
Benzodiazepine and Benzazepine Derivatives of 2-Methyl-1-phenylimidazo[4,5-c]pyridine

AUTHOR(S): Fray, M. Jonathan; Cooper, Kelvin; Parry, M. John; Richardson, Kenneth; Steele, John
CORPORATE SOURCE: Department of Discovery Biology, Pfizer Central Research, Sandwich/Kent, CT13 9NJ, UK
SOURCE: Journal of Medicinal Chemistry (1995), 38(18), 3514-23
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Following the discovery of moderately potent antagonist activity against platelet-activating factor (PAF) in 2-methyl-1-phenylimidazo[4,5-c]pyridine (IC50 = 840 nM) derivs. were prepared which incorporated various lipophilic groups attached to the Ph 4-position. Structure-activity relationships were evaluated where PAF antagonist activity was measured in vitro by determining the concentration of compound (IC50) required to inhibit the PAF-induced aggregation of rabbit washed platelets and in vivo by determining the oral dose (ED50) which protected mice from a lethal injection of PAF. [1,5]Benzodiazepines, e.g., (2,3-dihydro-1-methyl-4-[4-(2-methylimidazo[4,5-c]pyrid-1-yl)phenyl]-1H-[1,5]benzodiazepin-2-one) (IC50 = 4.9 nM, ED50 = 0.03 mg/kg po), were found to possess equivalent or superior potency to the 1,4-dihydropyridine PAF antagonist UK-74,505 [4-(2-chlorophenyl)-1,4-dihydro-3-(ethoxycarbonyl)-6-methyl-2-[4-(2-methylimidazo[4,5-c]pyrid-1-yl)phenyl]-5-[N-(2-pyridyl)carbamoyl]pyridine] in vitro and in vivo. Furthermore, a potent benzazepine, (7,8-dichloro-1-methyl-4-[4-(methylimidazo[4,5-c]pyrid-1-yl)phenyl]-2,3,4,5-tetrahydro-1H-1-benzazepin-2-one) (IC50 = 0.5 nM, ED50 = 0.03 mg/kg po), was discovered. These investigations prompted the synthesis and evaluation of addnl. diazepine derivs., which are described in the following paper. The relationship between the key PAF antagonist pharmacophores of 2-methyl-1-phenylimidazo[4,5-c]pyridine, a triazolothienodiazepine (WEB2170), and a pyrrolothiazolidine (RP-52,770) is discussed.

IT 167694-30-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazo[4,5-c]pyridine derivs. as platelet-activating factor antagonists)

RN 167694-30-6 HCAPLUS
CN Benzenebutanoic acid, α-[4-(2-methyl-1H-imidazo[4,5-c]pyridin-1-yl)benzoyl]-2-nitro-γ-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 20 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:549549 HCAPLUS
DOCUMENT NUMBER: 123:137091
TITLE: Structure-based design of human immunodeficiency virus-1 protease inhibitors. Correlating calculated energy with activity

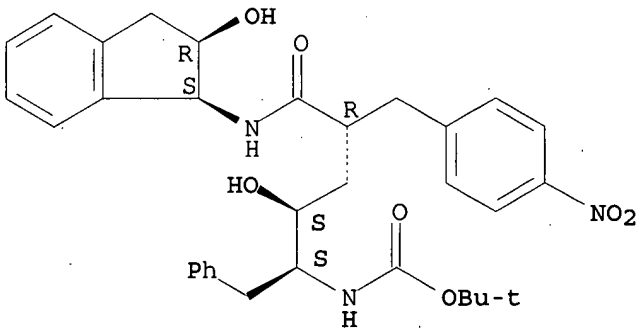
AUTHOR(S): Holloway, M. Katharine; Wai, Jenny M.
CORPORATE SOURCE: Molecular Systems Department, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: ACS Symposium Series (1995), 589(Computer-Aided Molecular Design), 36-50
CODEN: ACSMC8; ISSN: 0097-6156
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have found that a simple calculated energy value, Einter, correlates well with the observed in vitro enzyme activity of a series of HIV-1 protease inhibitors. This correlation was derived employing a test dataset of 33 inhibitors with modifications at the P1' and P2' sites. It has proved valuable in the structure-based design of subsequent HIV-1 protease inhibitors which exhibit significant structural variation. In particular, it has been successful in a truly predictive sense, i.e. predictions of activity were made prior to synthesis. Several examples of this are illustrated, including a precursor (41) to a current clin. candidate, L-735,524 (42).

IT 126410-15-9 126410-17-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(structure-based design of human immunodeficiency virus-1 protease inhibitors)

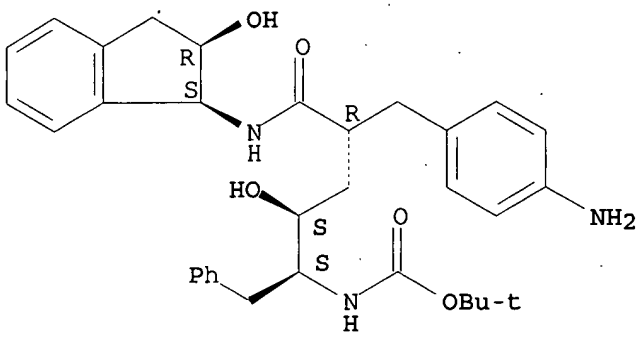
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



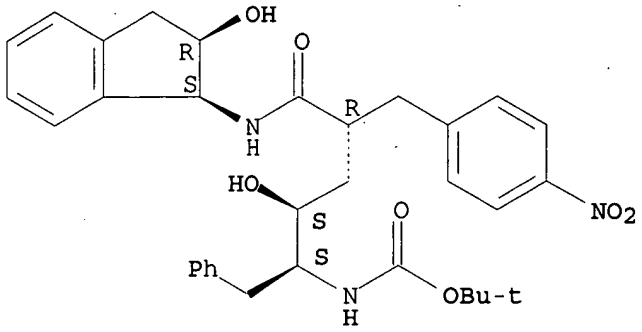
L4 ANSWER 21 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:297964 HCAPLUS
DOCUMENT NUMBER: 122:177664
TITLE: A priori prediction of activity for HIV-1 protease inhibitors employing energy minimization in the active site
AUTHOR(S): Holloway, M. Katharine; Wai, Jenny M.; Halgren, Thomas A.; Fitzgerald, Paula M. D.; Vacca, Joseph P.; Dorsey, Bruce D.; Levin, Rhonda B.; Thompson, Wayne J.; Chen, L. Jenny; et al.
CORPORATE SOURCE: Department of Molecular Systems, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: Journal of Medicinal Chemistry (1995), 38(2), 305-17
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A high correlation was observed between the intermol. interaction energy (Einter) calculated for HIV-1 protease inhibitor complexes and the observed in vitro enzyme inhibition. A training set of 33 inhibitors containing modifications in the P1' and P2' positions was used to develop a regression equation which relates Einter and pIC50. This correlation was subsequently employed to successfully predict the activity of proposed HIV-1 protease inhibitors in advance of synthesis in a structure-based design program. This included a precursor to the current phase II clin. candidate L-735,524. The development of the correlation, its applications, and its limitations are discussed, and the force field (MM2X) and host mol. mechanics program (OPTIMOL) used in this work are described.

IT 126410-15-9 126410-17-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(energy minimization in active site for design of HIV-1 protease inhibitors)

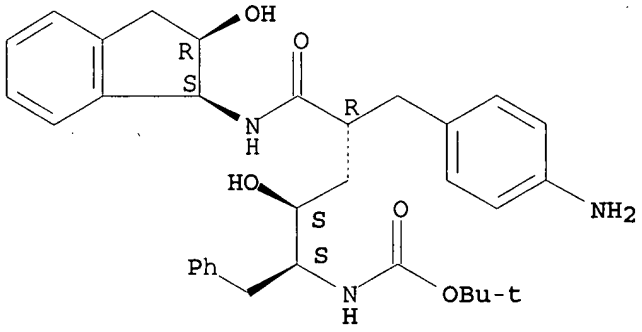
RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

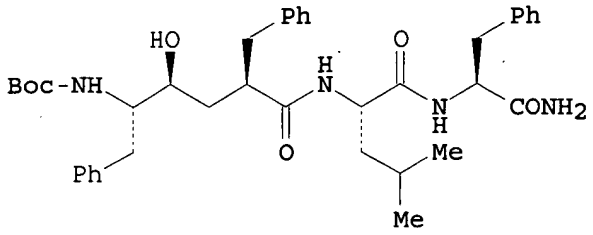


RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

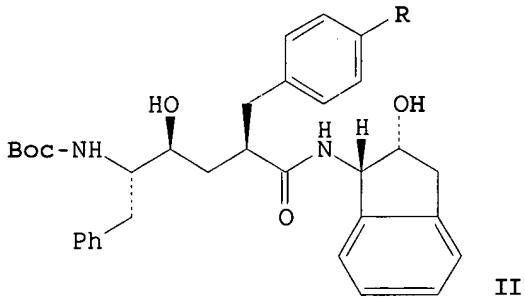
Absolute stereochemistry.



L4 ANSWER 22 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:408413 HCAPLUS
DOCUMENT NUMBER: 117:8413
TITLE: HIV-1 protease inhibitors based on hydroxyethylene dipeptide isosteres: An investigation into the role of the P1' side chain on structure-activity
AUTHOR(S): Young, Steven D.; Payne, Linda S.; Thompson, Wayne J.; Gaffin, Neil; Lyle, Terry A.; Britcher, Susan F.; Graham, Samuel L.; Schultz, Thomas H.; Deana, Albert A.; et al.
CORPORATE SOURCE: Dep. Med. Chem., Merck Sharp and Dohme Res. Lab., West Point, PA, 19486, USA
SOURCE: Journal of Medicinal Chemistry (1992), 35(10), 1702-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:8413
GI



I



II

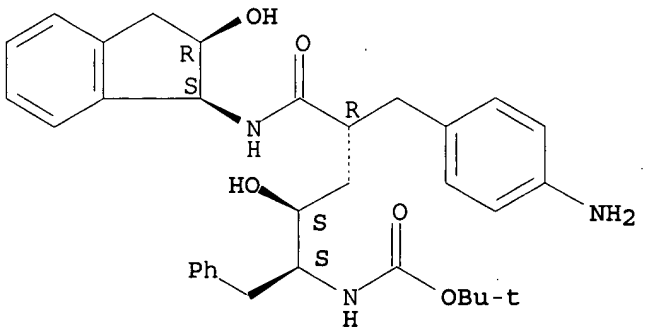
AB A systematic investigation was undertaken to determine the role of the P1' side chain in a series of hydroxyethylene isostere based inhibitors of HIV-1 protease. Substitution and homologation of the benzyl P1' side chain of the Phe-Phe isostere based pseudopeptides I (Boc = Me3CO2C) (L-682,679) and II (R = H) (L-685,434) with various heteroalkyl groups leads to a series of extremely potent inhibitors of the enzyme. Several examples of the most potent inhibitors were very effective in ex vivo cell based viral spread assay using human H9 T-lymphocytes and the the IIIb isolate of HIV-1. Compound II [R =(CH2)3OH] is 120 times more potent than I and 16 times more potent than II (R = H) in inhibiting the spread of infection in this assay.

IT 126410-17-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and inhibition by, of human immunodeficiency virus-1 protease)

RN 126410-17-1 HCAPLUS

CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

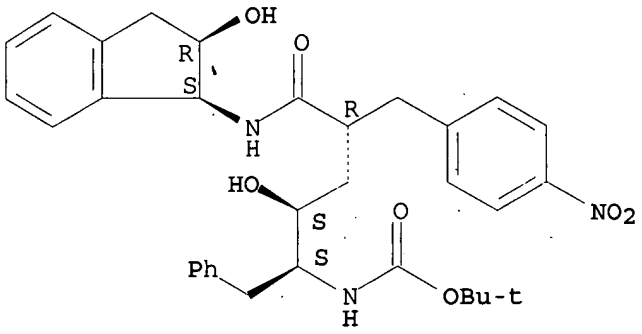


IT 126410-15-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 126410-15-9 HCAPLUS

CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 23 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1990:199132 HCAPLUS
DOCUMENT NUMBER: 112:199132
TITLE: Preparation of human immunodeficiency virus (HIV) protease inhibitors for treatment of AIDS
INVENTOR(S): Sigal, Irving S.; Huff, Joel R.; Darke, Paul L.; Vacca, Joseph P.; Young, Steven D.; Desolms, S. Jane; Thompson, Wayne J.; Lyle, Terry A.; Graham, Samuel L.; Ghosh, Arun K.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: Eur. Pat. Appl., 94 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

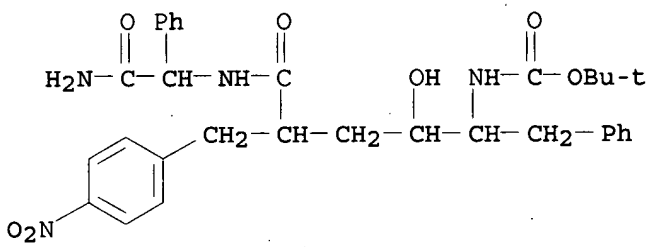
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 337714	A2	19891018	EP 1989-303539		19890411
EP 337714	A3	19910807			
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE					
FI 8901716	A	19891013	FI 1989-1716		19890411
NO 8901489	A	19891013	NO 1989-1489		19890411
ZA 8902627	A	19891129	ZA 1989-2627		19890411
DK 8901723	A	19891211	DK 1989-1723		19890411
AU 8932706	A1	19891019	AU 1989-32706		19890412
AU 620084	B2	19920213			
JP 02209854	A2	19900821	JP 1989-92762		19890412
PRIORITY APPLN. INFO.:			US 1988-180507	A	19880412
			US 1988-236084	A	19880824
			US 1989-328643	A	19890328

OTHER SOURCE(S): MARPAT 112:199132
GI For diagram(s), see printed CA Issue.
AB Dipeptides or amino acid amides or carboxamides A-G-B-B-J [I; A = Ph3C, H, CHO, (un)substituted C2-5 alkanoyl, phthaloyl, MeO2C, H2NOC(O), or arylsulfonylcarbamoyl, etc.; G = NHCHRCHR1QC(O), NHCHRQ1CHRC(:Z); Z = O, S, H2; R = H, OH, C1-4 alkoxy, NH2, etc.; R1 = OH, (un)substituted NH2; Q = (un)substituted C3-7 alicyclic, benzene, or 5- to 7-membered heterocyclic ring; Q1 = CH(OH)CHR, CH2NH, P(O)(OH)CH2, CH(OH), etc.; B = null, NHCHRC(:Z); J = OH, NH2, (un)substituted C1-6 alkoxy or C1-6

alkylamino, etc.], are prepared Thus, condensation of a hexanoic acid derivative (II; R2 = SiMe2CMe3, R3 = OH, BOC = Me3CO2C) (preparation given) with H-Leu-Phe-NH2.HCl.1/2H2O in the presence of 1-hydroxybenzotriazole.H2O, dimethyl-3-(3-dimethylaminopropyl)carbodiimide.HCl, and Et3N in DMF gave, after disilylation with Bu4NF in THF, II (R2 = H, R3 = Leu-Phe-NH2). The latter compound inhibited synthetic and Escherichia coli-expressed HIV protease with IC50 values of 2 and 0.6 nM, resp. Approx. 130 I were prepared

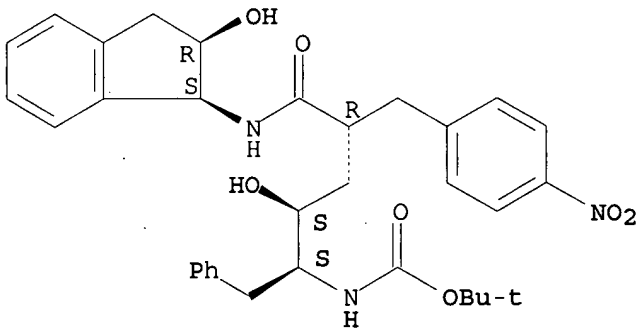
IT 126409-75-4P 126410-15-9P 126410-16-0P
126410-17-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as HIV protease inhibitor for AIDS treatment)

RN 126409-75-4 HCAPLUS
CN Carbamic acid, [5-[(2-amino-2-oxo-1-phenylethyl)amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

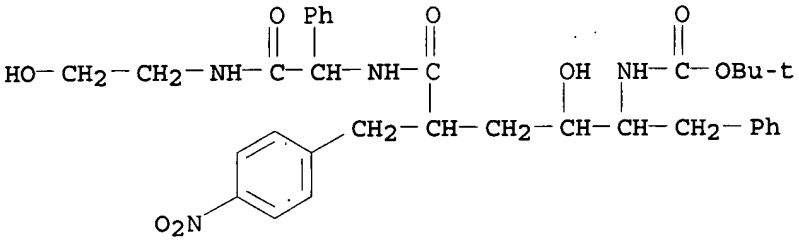


RN 126410-15-9 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

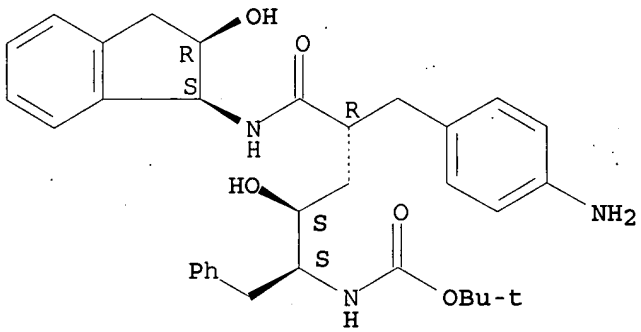


RN 126410-16-0 HCAPLUS
CN Carbamic acid, [2-hydroxy-5-[[2-[(2-hydroxyethyl)amino]-2-oxo-1-phenylethyl]amino]-4-[(4-nitrophenyl)methyl]-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

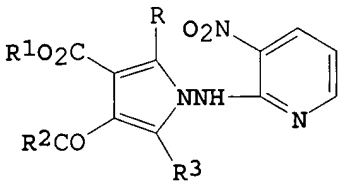


RN 126410-17-1 HCAPLUS
CN Carbamic acid, [(1S,2S,4R)-4-[(4-aminophenyl)methyl]-5-[[(1S,2R)-2,3-dihydro-2-hydroxy-1H-inden-1-yl]amino]-2-hydroxy-5-oxo-1-(phenylmethyl)pentyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

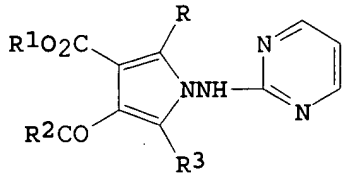
Absolute stereochemistry.



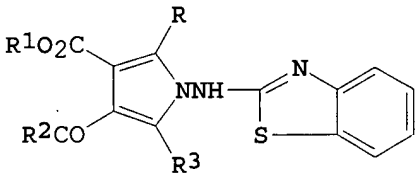
L4 ANSWER 24 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:102005 HCAPLUS
DOCUMENT NUMBER: 106:102005
TITLE: Effect of metal ions in organic synthesis. Part XXXI. Synthesis of new 3-carbonyl- and 3-carboxy-1-heterocyclaminopyrroles by copper(II) chloride-catalyzed reaction of heterocyclic azoalkenes
AUTHOR(S): Attanasi, Orazio; Filippone, Paolino; Mei, Amedeo; Serra-Zanetti, Franco
CORPORATE SOURCE: Fac. Sci., Univ. Urbino, Urbino, 61029, Italy
SOURCE: Journal of Heterocyclic Chemistry (1986), 23(1), 25-8
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:102005
GI



I



II



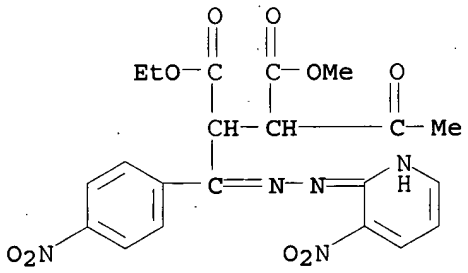
III

AB A new class of pyrroles I, II, and III (R = Me, 4-NO2C6H4; R1 = Me, Et, PhCH2; R2 = Me, Ph, OMe, OEt, OCH2Ph; R3 = Me, Ph, 4-O2NC6H4) were prepared by copper(II) chloride-catalyzed reaction heterocyclic conjugated azoalkanes with R2COCH2COR3.

IT 106997-87-9P 106997-88-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring closure of, cupric chloride as catalyst for)

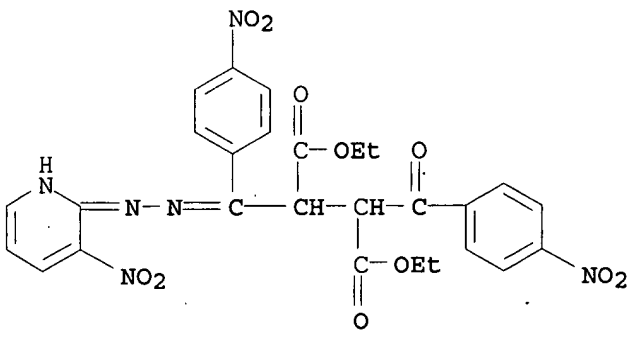
RN 106997-87-9 HCAPLUS

CN Butanedioic acid, 2-acetyl-3-[(4-nitrophenyl)[(3-nitro-2-pyridinyl)hydrazono]methyl]-, 4-ethyl 1-methyl ester (9CI) (CA INDEX NAME)

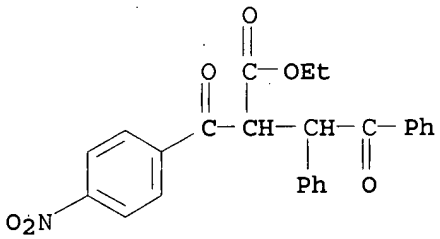


RN 106997-88-0 HCAPLUS

CN Butanedioic acid, 2-(4-nitrobenzoyl)-3-[(4-nitrophenyl)[(3-nitro-2-pyridinyl)hydrazono]methyl]-, diethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 25 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:419471 HCAPLUS
DOCUMENT NUMBER: 77:19471
TITLE: 1,3-Dipolar cycloadditions. 62. Benzonitrile 4-nitrobenzylide and its reactions with carbon-carbon double and triple bonds
AUTHOR(S): Huisgen, Rolf; Stangl, Heinz; Sturm, Hans J.; Raab, Rainer; Bunge, Karlheinz
CORPORATE SOURCE: Inst. Org. Chem., Univ. Muenchen, Munich, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1972), 105(4), 1258-78
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.
AB The 1st representative of the class of nitrile ylides, benzonitrile 4-nitrobenzylide, was generated in a small equilibrium concentration from PhCCl:NCH2C6H4NO2-p by HCl elimination with NEt3. Cycloaddns. with HC.tplbond.CCO2Me, PhC.tplbond.CCO2Et, and MeO2CC.tplbond.CCO2Me in situ gave 3,4-disubstituted 2-phenyl-5-(p-nitrophenyl)-pyrroles (I), whereas reactions with CH2:)CHCO2Me, CH2:CHCN, and norbornene gave pairs of diastereomeric 1-pyrrolines in good yields. Di-Me fumarate, 1,4-naphthoquinone, and acenaphthylene were used as further dipolarophiles.
IT 36710-13-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36710-13-1 HCAPLUS
CN Benzenebutanoic acid, α-(4-nitrobenzoyl)-γ-oxo-β-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 26 OF 26 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1955:4684 HCAPLUS
DOCUMENT NUMBER: 49:4684
ORIGINAL REFERENCE NO.: 49:959a-e
TITLE: Conditions of reaction and condensation of aldehydes and ketones with α-ketonic acids
AUTHOR(S): Cordier, P.
CORPORATE SOURCE: Fac. pharm., Strasbourg
SOURCE: Bulletin de la Societe Chimique de France (1953), (No. 10), C37-40
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB The condensation of phenylpyruvic acid (I) and its derivs. with aldehydes and ketones were studied. When I is condensed with benzaldehyde (II), the final product is O.CO.CO.CHPh.CHPh. p-Nitrophenylpyruvic ester (III) was

prepared from p-nitrotoluene and Et oxalate. Two geometric isomers of the enol of III (m. 106° and 120°) were obtained. Hydrolysis of both isomers yielded p-nitrophenylpyruvic acid, m. 194°. When the lower melting isomer of III enol is condensed with furfural (IV), II, anisaldehyde (V), or cinnamaldehyde in alc. alkali, the corresponding keto lactones are obtained, m. 201°, 236°, 271°, and 207°, resp. With α-naphthaldehyde, 2 isomers, m. 215° and 223°, are gotten. When the enol of III, m. 120°, is treated under the same conditions, hydrocarbons, p-O2NC6H4CH:CHR, are obtained. When the reaction is carried out in an acid medium, both isomers yield the keto lactone. p-Methoxyphenylpyruvic acid (VI), m. 183°, was prepared from p-MeOC6H4CH2CN and (CO2Et)2, followed by hydrolysis and decarboxylation. Condensation of VI with II yields isomeric keto lactones, m. 170° (VII), and m. 180° (VIII); heating transforms VII to VIII. A hydroxy acid, m. 83°, can be prepared from VII. The reaction between VI and V yields two lactones, m. 106°, and m. 107° (IX). The Me and Et esters of VI, when condensed with II or V yield VII and IX, resp. Condensation of VI and IV yields one lactone, m. 181°. p-Bromophenylpyruvic acid (X), m. 198°, and II yield a lactone, m. 212°. The lactone resulting from V and X melts at 201°. The reaction between I and aliphatic Me ketones yields C6H4CHC(OH)(CH2OR)CO2H. Aromatic Me ketones when treated with III yield a dimer of III. The latter lactonizes to O.CO.CO.CH(C6H4NO2-p).C(CO2H)(CH2C6H4-p). Two isomers, m. 135° and 193°, of this lactone were isolated. Ethylenic ketones, such as PhCH:CHAc, and I give cyclic ketones, as CO.CH2.C(OH)(CO2H).CHPh.CHPh.CH2. The compound formed from I and benzalacetophenone, m. 225° and that formed from the p-MeO derivative, m. 208°.

IT 859306-70-0P, Glutaric acid, 2-hydroxy-2-p-nitrobenzyl-3-(p-nitrophenyl)-4-oxo-
RL: PREP (Preparation)
(preparation of)

RN 859306-70-0 HCAPLUS

CN Glutaric acid, 2-hydroxy-2-p-nitrobenzyl-3-(p-nitrophenyl)-4-oxo- (5CI) (CA INDEX NAME)